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49th International Symposium on Essential Oils (ISEO2018)
Book of Abstracts


UNIVERSITY OF NIŠ

## INSTRUCTIONS FOR CONTRIBUTORS

**Contributions** should be (preferably) in English, French or German.
Under the paper title, the name(s) of the author(s) should be given while the full name, official title, institute or company affiliation and the like should be placed at the end of the paper together with the exact mail and e-mail address, as well as short (running) title of paper.
**Manuscript format.** A brief abstract of approximately 100 to 150 words in the same language and a list of up to six key words should precede the text body of the manuscript. All the authors apart from foreign ones should also submit a complete manuscript in Serbian. Manuscripts should be prepared as doc. file, Word version 6.0 or higher. Manuscript should be prepared using a Word template (downloaded from web address http://casopisi.junis.ni.ac.rs/index.php/FUPhysChemTech/about/submissions#onlineSubmissions).
**Manuscript length.** Brief articles and discussions (10 pages or less) are encouraged. Otherwise, papers should present well-focused arguments of approximately 16 pages.
**Style requirements**. **Letters, figures and symbols** should be clearly denoted.
**Equations** should be typewritten and, with the number, placed in parentheses at the right margin. References to equations should be in the form "Eq. (2)" or simply (2). For equations that cannot be entered in a single line, use the Equation Editor in MS Word. In equations and in the text, *italicize* symbols that are used to represent variables or parameters, including subscripts and superscripts. Only use characters and symbols that are available in the Equation Editor, in the *Symbol font* or in *Times New Roman*.
**All illustrations (figures, photographs, line drawings, graphs)** should be numbered in series and all legends should be included at the bottom of each illustration. All figures, photographs, line drawings and graphs, should be prepared in electronic form and converted in TIFF or JPG (max quality) file types, in 300 dpi resolution, for superior reproduction. Figures, line drawings and graphs prepared using elements of MS Drawing or MS Graph must be converted in form of pictures and unchangeable. All illustrations should be planned in advance so as to allow reduction to 12.75 cm in column width. Please review all illustrations to ensure that they are readable.
All **tables** should be numbered with consecutive Arabic numbers. They should have descriptive captions at the top of each table and should be mentioned in the text.
The **references** should be numbered in the order in which they appear in the text, at the end of the manuscript, in the same way as the following examples (for a book, a paper in a journal, paper in a contributed volume and for an unpublished paper):

*Serial:*

C.A. Hunter and J.K.M. Sanders, The nature of π-π interactions, *Journal of the American Chemical Society*, **112** (14), 5525-5534 (1990).

*Book:*

R.P. Adams, *Identification of essential oil components by gas chromatography/mass spectroscopy*, Allured Publishing Corporation, Illinois, 2007.

*Book, part of:*

G.R. Mettam, L.B. Adams, 2009. How to prepare an electronic version of your article, in: B.S. Jones, R.Z. Smith (Eds.), Introduction to the Electronic Age. E-Publishing Inc., New York, pp. 281–304.

*Conference proceedings:*

A. Holmes-Siedle, L. Adams and G. Ensell, MOS dosimeters-improvement of responsivity, *Proc. 1st European Conf. on Radiation and its Effects on Devices and Systems (RADECS 91), Montpellier, France*, 1991, pp. 65-69.

*Bulletin or Reports:*

R.M. Perkin, 1999. *Feature models in Virtual Product Development*, Report ECRC/M1677, Capenhurst, England.

*Thesis:*

M.L. Reed, *Si-$SiO_2$ interface trap anneal kinetics*, Ph. D. Thesis, Stanford University, Stanford, 1987.

*Patents:*

R. Wu, 1982. *Drying Systems*, US Patent No. 4359826.

*Others:*

D. Zlatković, 2014, *Volatile secondary metabolites from* Ferula ovina, unpublished paper (or private communication).

*World wide web page*

M. Grossman (5 September 2001). *Technology and Diplomacy in the 21st Century*, [Online], U.S. Department of State. Available from: <http://www.state.gov/p/6580.htm> [21 May 2004].

*Software*

Accelrys Software Inc., 2013. Discovery Studio Visualizer, Release 4.0, San Diego: Accelrys Software Inc.

References should be quoted in the text by the corresponding number in square brackets.

**Electronic submission**. Papers for consideration should be submitted to the Series Editor in electronic form via the Journal's home page: http://casopisi.junis.ni.ac.rs/index.php/FUPhysChemTech/index.

**FACTA UNIVERSITATIS**
Series: **Physics, Chemistry and Technology** Vol. 16, Nº 1, Special Issue, 2018, p. 1
49th International Symposium on Essential Oils (ISEO2018) • Book of Abstracts

49th ISEO

## WELCOME

On behalf of the Organizing Committee, it is my great pleasure to welcome you to the 49th International Symposium on Essential Oils (ISEO2018).

Over the years, this prestigious annual symposium has developed into a unique meeting arena between leading experts, academic and industry scientists involved in the essential-oil research and representatives of the essential-oil industry from all around the world. The 49th ISEO will feature plenary lectures and presentations of cutting-edge science of essential oils from a diverse group of scientists in the fields of natural product isolation, organic synthesis, chemometrics, chemical biology, biosynthesis, pharmacology and analytical methodology development. Recent advances and future trends in the application of essential oils and their constituents in the fragrance industry, pharmacy, cosmetology, food production and agriculture will be highlighted, as well. The meeting will provide opportunities for in-depth scientific discussions and sharing unpublished results in both formal and informal settings.

Although ISEO symposia have a tradition of nearly half a century, it will take place in Serbia for the first time. Niš is the third largest city in Serbia, situated on the river of Nišava and represents a cultural, economic, administrative, business and university center of southeastern Serbia. For centuries, an important geographical and strategic position of the town has determined its destiny, so this region was inhabited by the Romans, Goths, Illyrians, Celts, Ottomans, Slavs, etc. Alongside rich cultural and historical heritage, southeastern Serbia has a unique natural beauty with two stunning gorges surrounded by picturesque Suva planina mountain characterized by exceptional biological diversity.

Many geographers, travelers, and historians considered the city of Niš as a gateway between the East and West, and we will set this as our main goal–to unify scientists from universities, research centers and industry from all over the world and to join different cultures and knowledge together.

ISEO2018 abstracts are published in the Special Issue of *Facta Universitatis: Series Physics, Chemistry and Technology*, a scientific journal published by the University of Niš since 1986. The outstanding contributions presented at the ISEO2018 Symposium (plenary lectures, oral and poster presentations) will enjoy the opportunity of having their full work published in the *Food & Chemical Toxicology* Special Issue dedicated solely to the "Toxicity of essential oils and their constituents".

I wish all of the ISEO2018 participants a highly successful and enjoyable symposium and many unforgettable memories of your stay in Niš, Serbia. Thank you for joining us at this meeting!

*Dr Niko Radulović*
*The President of the ISEO2018 Organizing Committee*

## *ISEO2018 Organizing Committee*

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## *ISEO Permanent Scientific Committee*

## ISEO2018 ORGANIZERS

**Serbian Society for Phytochemistry and Phytomedicine**

**Organic synthesis and analysis group**

**University of Niš**

**Faculty of Sciences and Mathematics, University of Niš**

**The Republic of Serbia**
**Ministry of Education, Science and Technological Development**

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**International Federation of Essential Oils and Aroma Trades**

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## YOUNG SCIENTISTS FELLOWSHIP

Thanks to the generous support of the International Federation of Essential Oils & Aroma Trade (IFEAT), the ISEO2018 Organizing Committee offered Registration Fellowships to 20 selected young scientists who submitted a presentation in ISEO2018. The Registration Fellowships award consists of the registration fee reimbursement and the awardees will also receive a certificate.

As a result of this generosity, the supported young scientists are now able to contribute to the development of the essential oils and natural volatiles research field. There is also an excellent possibility to bring together the next generation of scientists and experts from around the world enabling them to share experiences and to develop new ideas.

After an intense evaluation and selection procedure, the Organizing Committee of ISEO2018 has accepted twenty contributions. Among them, nine were chosen for oral presentations and the remaining twelve were accepted for poster presentations.

The International Federation of Essential Oils & Aroma Trade (IFEAT) and the ISEO2018 Organizing Committee supported the registration fees of the following young scientists:

| | |
|---|---|
| **Verica Aleksić Sabo** | *University of Novi Sad*, Serbia |
| **Carmen M. S. Ambrosio** | *São Paulo University*, Brazil |
| **Ina Aneva** | *Bulgarian Academy of Sciences*, Bulgaria |
| **Leidy J. A. Ferro** | *University of Pécs*, Hungary |
| **Eleni Fitsiou** | *Democritus University of Thrace*, Greece |
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| **Asit Ray** | *Siksha O Anusandhan University*, India |
| **Elwira Sieniawska** | *Medical University of Lublin*, Poland |
| **Filomena Silva** | *University of Zaragoza*, Spain |
| **Milica Stevanović** | *University of Niš*, Serbia |
| **Musa Türkmen** | *Mustafa Kemal University*, Turkey |
| **Ayaka Uehara** | *Université Côte d'Azur*, France |
| **Margita Utczás** | *University of Physical Education*, Hungary |
| **Dragan Zlatković** | *University of Niš*, Serbia |
| **Milena Živković** | *University of Niš*, Serbia |

# GENERAL INFORMATION

## *Symposium venue*

**1)** University rectorate building–Banovina (*plenary and invited lectures, and oral presentations*)
Univerzitetski trg 2, 18000 Niš, Serbia
tel: +381 18 257 970 and +381 18 257956
www.ni.ac.rs

**2)** showroom Oficirski dom (*poster sessions*)
Orlovića Pavla 28a, 18000 Niš, Serbia

**3)** New City Hotel (*symposium lunches*)
Vožda Karađorđa 12, 18000 Niš, Serbia
tel: +381 18 504 800
www.newcityhotelnis.com


## *Website*

You will find the latest details about the Symposium on the website at http://iseo2018.com/.

## Registration

The registration desk will be located in the entrance of the University rectorate building (Banovina) or Oficirski dom showroom according to the following schedule:

| | | |
|---|---|---|
| Thursday, September 13 | 16.00–19.00 | *Oficirski dom showroom* |
| Friday, September 14 | 08.00–17.00 | *University rectorate building* |
| Saturday, September 15 | 08.00–17.00 | *University rectorate building* |
| Sunday, September 16 | 08.00–12.30 | *University rectorate building* |

## Symposium Language

The official language of the symposium is English. There will be no simultaneous translation.

## Badges

All participants and accompanying persons will receive a personal badge upon registration. Delegates are kindly requested to wear their name badge when attending the meetings or social events.

## Exhibition

In accordance with the conventions of the symposium, parallel to the scientific sessions a professional exhibition is to be organized in the University rectorate building and the Oficirski dom showroom. The exhibition will be open during the whole scientific programme.

## Meals

Lunches on Friday, Saturday and Sunday are included in the registration fee. Lunches will be served in the New City Hotel between 13.00-14.30 on Friday, between 12.50-14.15 on Saturday, and between 13.30-14.45 on Sunday.

## Liability and Insurance

The participants are advised to arrange their own insurance for health, travel, and property. The organizers cannot accept liability for any personal accidents, loss of belongings or damage to private property of participants and accompanying persons that may occur during the symposium.

## *Plenary and Invited Lectures and Oral Presentations*

The length of plenary lectures and oral presentations are limited to 45 and 20 min. Invited speakers have 30 min for their presentations. The organizers advise leaving 5 (plenary and invited) or 3 (oral) min for questions and discussion. The organizers kindly ask a strict adherence to the agreed time, as the session chairs will be asked to rigorously maintain the time schedule. PowerPoint or PDF presentations are accepted on USB sticks. Version MS PowerPoint 2003-2010 is recommended. Laptops and projectors will be available for the presenters. The presentation has to be copied to the laptop/computer a day ahead or in the coffee break before the beginning of the session.

## *Poster Presentations*

Posters will be exhibited according to their designated numbers in the book of abstract. Odd (PP1, PP3, PP5, etc.) and even (PP2, PP4, PP6, etc.) numbered posters will be displayed on Friday and Saturday, respectively. The recommended size for the poster is about the standing A0 standard (ca. 84 × 119 cm). The organizers will provide all equipment and tools (pins, adhesive tape, and scissors) to mount your poster to the board at the conference venue. Poster presenters are kindly requested to remove their posters after each poster session. The authors should stand by their posters and be available to discuss their research during the poster session.

## *Best Poster Award*

Three poster presentations will be recognized for excellence at ISEO2018. Selection, by an Awards committee, will be based on subject matter, quality of presentation and research, oral delivery, and visual impact. The winners of the Best Poster Award will be announced during the Closing Ceremony of the 49th ISEO Symposium. The monetary prize for the first, second, and third place will be 200, 150, and 100 €, respectively. All winning authors will also receive award certificates.

## SOCIAL PROGRAMMES

### *Welcome Reception*

The Welcome reception will be served on September 13th (from 19.00 to 21.00) at the historical building showroom Oficirski dom located in the historical heart of the city of Niš. Music will be provided by a local group of performers. The Welcome reception is included in the registration fee.

### *Gala Dinner*

Gala dinner will be held on September 15th (from 19.30 to 24.00) at a century-old wine cellar Malča, located about 15 km from Niš, where you will discover local winemaking tradition and cuisine. Music will be provided by a local band. Bus transportation is provided and gathering will be at 19.00 in front of the University rectorate building. The symposium dinner is not included in the registration fees but should be booked during the online registration.

### *Half-day Excursion*

A half-day excursion will be organized on September 16th and it will consist of visits to the sights of the city of Niš accompanied by a certified guide. Bus transportation is provided and gathering will be at 15.00 in front of the University rectorate building. The excursion is included in registration fee, but advanced application (during registration) is required.

## SCIENTIFIC PROGRAMME

| | | |
|---|---|---|
| **13th September 2018, Thursday** | | |
| 16.00-19.00 | **Registration** | *University rectorate building* |
| 19.00-21.00 | **Welcome reception** | *Officirski dom showroom* |
| **14th September 2018, Friday** | | |
| 08.00-09.30 | **Registration** | *University rectorate building* |
| 09.30-10.10 | **Opening Ceremony** | *University rectorate building* |
| **Session I** | Chairs: | Agnieszka Ludwiczuk (Lublin, Poland) |
| **10.10-12.25** | | Niko Radulović (Niš, Serbia) |
| 10.10-10.55 | **PL1** | **Nicolas Baldovini** (Nice, France)<br>*"Applying organic synthesis in the analysis of essential oils"* |
| **10.55-11.15** | **Coffee break** | |
| 11.15-11.45 | **IS1** | **Yoshinori Asakawa** (Tokushima, Japan)<br>*"Highly efficient production of functional substances from synthetic compounds and secondary metabolites by mammal and microbial biotransformation"* |
| 11.45-12.05 | **OP1** | **Petras Rimantas Venskutonis** (Kaunas, Lithuania)<br>*"Essential oils from 11* Cannabis sativa *cultivars isolated by different methods and toxicological evaluation of their components"* |
| 12.05-12.25 | **OP2** | **Margita Utczás** (Budapest, Hungary)<br>*"Novel analytical tool for a univocal flavor and fragrance identification: Gas chromatography coupled with condensed-phase FTIR and TOF mass spectrometry"* |
| **13.00-14.30** | **Lunch** | ***New City Hotel*** |
| **Session II** | Chairs: | Yoshinori Asakawa (Tokushima, Japan) |
| **14.30-16.35** | | Nicolas Baldovini (Nice, France) |
| 14.30-15.15 | **PL2** | **Daniel Strub** (Wrocław, Poland) and<br>**Stanislaw Lochynski** (Wrocław, Poland)<br>*"Stereochemistry of volatiles–the status and perspectives"* |
| 15.15-15.35 | **OP3** | **Györgyi Horváth** (Pécs, Hungary)<br>*"Applicability of cinnamon bark essential oil in respiratory tract diseases–from* in vitro *to* in vivo *experiments"* |
| 15.35-15.55 | **OP4** | **Huong Thi Nguyen** (Budapest, Hungary)<br>*"Changes in the volatile compounds of two wormwood (*Artemisia absinthium *L.) accessions under controlled weather conditions"* |
| 15.55-16.15 | **OP5** | **Ewa Maciejczyk** (Łódź, Poland)<br>*"Juniper berry (*Juniperus communis *L.) supercritical extract, essential oil and absolute comparison"* |
| 16.15-16.35 | **SP1** | **Presentation of the sponsor:**<br>**Neža Rangus** (ARXFARM d.o.o., Slovenia)<br>Helichrysum *oil from the Balkan peninsula* |
| **17.00-18.30** | **Poster Session I and Coffee Break** | Odd numbers (like PP1, PP3, PP5, etc.)<br>*Oficirski dom showroom* |
| **19.00-** | **ISEO Permanent Scientific Committee meeting** | |

| **15th September 2018, Saturday** | | |
|---|---|---|
| **Session III** | Chairs: | Luigi Mondello (Messina, Italy) |
| **09.00-10.55** | | Stanislaw Lochynski (Wrocław, Poland) |
| 09.00-09.45 | **PL3** | **Agnieszka Ludwiczuk** (Lublin, Poland)<br>*"Bryophyte volatiles: chemical diversity, chemotaxonomic significance and biological activity"* |
| 09.45-10.15 | **IS2** | **Gordana Stojanović** (Niš, Serbia)<br>*"Static headspace GC-MS analysis* versus *GC-MS analysis of essential oils"* |
| 10.15-10.35 | **OP6** | **Isiaka A. Ogunwande** (Lagos, Nigeria)<br>*"Chemical constituents, antiinflammatory and antinociceptive activities of essential oils from* Cordia millenii, Bougainvillea glabra *and* Phyllanthus muellerianus*"* |
| 10.35-10.55 | **OP7** | **Guy Kamatou** (Pretoria, South Africa)<br>*"An overview of the biological activities and essential-oil composition of three South African* Salvia *species"* |
| **10.55-11.15** | **Coffee break** | |
| **Session IV** | Chairs: | Humberto Bizzo (Rio de Janerio, Brazil) |
| **11.15-12.50** | | Johannes Novak (Vienna, Austria) |
| 11.05-11.50 | **PL4** | **Luigi Mondello** (Messina, Italy)<br>*"Linear retention index approach applied to liquid chromatography coupled to PDA and QqQ MS detectors for reliable characterization of oxygen heterocyclic compounds in essential oils and finished cosmetic products"* |
| 11.50-12.10 | **OP8** | **Carmen M.S. Ambrosio** (São Paulo, Brazil)<br>*"Chemical composition, antibacterial and antioxidant activity of a citrus essential oil and its fractions"* |
| 12.10-12.30 | **OP9** | **Ayaka Uehara** (Nice, France)<br>*"Characterization of the odorant constituents of* Helichrysum italicum *essential oil"* |
| 12.30-12.50 | **OP10** | **Filomena Silva** (Zaragoza, Spain)<br>*"Cyclodextrin nanosponges as a new encapsulating agent for essential oils and their effectiveness against foodborne pathogens"* |
| **12.50-14.15** | **Lunch** | ***New City Hotel*** |
| **Session V** | Chairs: | Jan Karlsen (Oslo, Norway) |
| **14.15-16.20** | | Hüsnü Can Başer (Eskisehir, Turkey) |
| 14.15-15.00 | **PL5** | **Michael Keusgen** (Marburg, Germany)<br>*"Volatile compounds of the genus* Allium *L."* |
| 15.00-15.20 | **SP2** | **Presentation of the sponsor:**<br>**Nikunj Harlalka** (Sankhubaba International, India)<br>*"Community-based production and organic certification of aromatic & medicinal crops in India"* |
| 15.20-16.20 | **WS** | **Workshop:**<br>**Dragan Zlatković** (Niš, Serbia)<br>*"GC-MS made easy: AMDIS in the analysis of complex mixtures of volatiles"* |

| | | |
|---|---|---|
| **16.30-18.00** | **Poster Session II and Coffee Break** | Even numbers (like PP2, PP4, PP6, etc.) *Oficirski dom showroom* |
| **19.00-24.00** | **Gala Dinner** | *Wine cellar Malča* |

## 16th September 2018, Sunday

| | | |
|---|---|---|
| **Session VI** | Chairs: | Éva Németh-Zámboriné (Budapest, Hungary) |
| **9.00-10.35** | | Fatih Demirci (Eskisehir, Turkey) |
| 09.00-09.45 | **PL6** | **Ioanna Chinou** (Athens, Greece) *"The regulatory framework for the quality and safe use of essential oils as herbal medicinal products. Selected examples from our Balkan "neighborhood"* |
| 09.45-10.15 | **IS3** | **Neda Mimica-Dukić** (Novi Sad, Serbia) *"Therapeutic efficiency of essential oils against* Helicobacter pylori *infection"* |
| 10.15-10.35 | **OP11** | **Milica Pejčić** (Niš, Serbia) *"Inhibitory effects of* Ocimum basilicum *and* Salvia officinalis *essential oils on virulence factors of* Pseudomonas aeruginosa *clinical isolates"* |
| **10.35-11.00** | **Coffee break** | |
| **Session VII** | Chairs: | Patrizia Rubiolo (Turin, Italy) |
| **11.00-13.30** | | Györgyi Horváth (Pécs, Hungary) |
| 11.00-11.45 | **PL7** | **Fabio Boylan** (Dublin, Ireland) *"Pharmacologically active derivatives of anthranilic acid occurring naturally in essential oils"* |
| 11.45-12.05 | **OP12** | **Nikola Stojanović** (Niš, Serbia) *"Evidences for lemon-balm essential oil suppression of anxiety-related behavior in animal and* in vitro *models"* |
| 12.05-12.20 | **OP13** | **Leidy J. A. Ferro** (Pécs, Hungary) *"Cytotoxicity and the effect on the inflammation response of thyme oil and thymol: evaluation in human macrophage cells"* |
| 12.20-12.40 | **OP14** | **Jacek Łyczko** (Wrocław, Poland) *"The Jerusalem Balsam–a case study of a 150-year-old sample"* |
| 12.40-13.00 | **OP15** | **Elwira Sieniawska** (Lublin, Poland) *"Microemulsions of essential oils – an improvement of solubility or something more?"* |
| **13.00-13.30** | **Closing Ceremony** | |
| **13.30-14.45** | **Lunch** | ***New City Hotel*** |
| **15.00-19.00** | **Half-day Excursion** | |

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49th ISEO

# PLENARY LECTURES

| | | |
|---|---|---|
| **PL1** | *Nicolas Baldovini* (France) | **Applying organic synthesis in the analysis of essential oils** |
| **PL2** | *Daniel Jan Strub* (Poland) | **Stereochemistry of volatiles–the status and perspectives** |
| **PL3** | *Agnieszka Ludwiczuk* (Poland) | **Bryophyte volatiles: chemical diversity, chemotaxonomic significance and biological activity** |
| **PL4** | *Luigi Mondello* (Italy) | **Linear retention index approach applied to liquid chromatography coupled to PDA and QqQ MS detectors for reliable characterization of oxygen heterocyclic compounds in essential oils and finished cosmetic products** |
| **PL5** | *Michael Keusgen* (Germany) | **Volatile compounds of the genus *Allium* L.** |
| **PL6** | *Ioanna Chinou* (Greece) | **The regulatory framework for the quality and safe use of essential oils as herbal medicinal products. Selected examples from our Balkan "Neighbourhood"** |
| **PL7** | *Fabio Boylan* (Ireland) | **Pharmacologically active derivatives of anthranilic acid occurring naturally in essential oils** |

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## PL1. Applying organic synthesis in the analysis of essential oils

*Nicolas Baldovini*[1]*

*Keywords*: essential oil analysis, organic synthesis, combinatorial synthesis, mass spectral and retention indices databases

Nowadays, the analysis of essential oils (EOs) is usually realized by the use of Gas Chromatography coupled with Mass spectrometry (GC-MS). Indeed, a significant part of the present knowledge on EOs comes from this ingenious association of a highly resolutive separation technique (GC) with the sensitive and informative detection by mass spectrometry. Interesting advances have been proposed to push the boundaries of classical GC techniques (using for example even more resolutive multidimensional GC) or to improve the sensitivity of MS detectors. However, one of the main limitations of this system is linked to the databases used for the identification of the analytes. Hence, the performance of the analysis depends on the reliability and the wealth of information contained in the libraries of mass spectra and retention indices used to identify the constituents. General commercial databases are not always adapted to the characterisation of EO components and the constitution of homemade libraries of authentic compounds is a long and expensive task. In many cases, organic synthesis can be of a great help to address such issues of EO analyses. Hence, the conversion of EO constituents by simple synthetic transformations (hemisynthesis), or even the total synthesis of some components can bring extremely useful information to confirm the identifications. Combinatorial synthesis is another very rapid and useful approach for the preparation of mixtures of homologues which can be used as such to enrich GC-MS libraries as the components of homologous series are usually perfectly resolved on apolar columns. Specific EOs analyses (enantiomeric analyses, characterization of key odorants) are also nicely helped by the syntheses of potent odorants and of racemic and/or enantiopure constituents.

In this presentation, we will describe some of our studies on various EOs and extracts of natural volatiles (sandalwood, vetiver, frankincense, Atlas cedarwood, *Helichrysum* and *Daucus* species etc.) where organic synthesis played a key role for the identification of their constituents and a better characterization of their properties. We hope to convince the community of scientists working in the field of EO analysis that many common problems can be easily solved by simple synthetic procedures which do not necessarily require advanced knowledge or sophisticated equipment.

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## PL2. Stereochemistry of volatiles–the status and perspectives

*Daniel Jan Strub*[1]*, Stanisław Lochyński[1]

*Keywords*: stereochemistry, fragrance chemistry and technology, fine chemicals

Stereochemistry is an important subject in various areas of fundamental chemistry, chemical-producing industries, medicine, and life in general. A huge effort has been undertaken over the last century to analyze and synthesize complex natural and synthetic compounds [1].

Optically pure plant-derived low-molecular compounds are important raw materials for the development of potential new products for the flavor and fragrance (F & F) industry [2,3]. Nowadays, studies towards innovations in the F & F field are focused not only on one new molecule but preferably on the whole process related to that molecule's production. Modern approaches in optically pure compound preparation involve the use of enzymes, whole-cell native and bioengineered microorganisms instead of toxic chemical catalysts, maximal atomic economy over the synthetic route, and a shift from batch to flow processes.

This presentation will provide a brief overview of modern "green" approaches in the F & F field with emphasis on the stereochemical processes involved in F & F development.

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## PL3. Bryophyte volatiles: chemical diversity, chemotaxonomic significance and biological activity

*Agnieszka Ludwiczuk*[1]*, Yoshinori Asakawa[2]

*Keywords*: bryophytes, liverworts, oil bodies, terpenoids, chemotaxonomy

Bryophytes are spore-forming plants, which occupy a position in the plant kingdom in between algae and pteridophytes. These are divided into three classes, mosses, liverworts, and hornworts [1]. Phytochemistry of bryophytes has been neglected for a long time because they are morphologically very small and it is difficult to collect a sufficient amount of plant material for study. The second problem is proper identification of plant material, which is especially challenging, because of their small size, their often microscopic or chemical distinguishing features [1-3]. Among the bryophytes, the chemical constituents of the Marchantiophyta and their biological activity have been studied in the most detail. Liverworts are characterized by the presence of oil bodies, unique organelles in which terpenoids and aromatic compounds are accumulated. Many of these compounds have unprecedented structures, and some, including the pinguisane-type sesquiterpenoids and sacculatane-type diterpenoids, have not been found in any other plants, fungi or marine organisms. A characteristic structural phenomenon of liverwort constituents is that most sesqui- and diterpenoids are enantiomers of those found in higher plants [1-3]. Constituents occurring in liverworts exhibit interesting biological activities, such as antibacterial, antifungal, cytotoxic, insect repellent, as well as some enzyme inhibitory and apoptosis-inducing activities [1,4]. The second very important direction of research concerning liverwort chemistry is the chromatographic fingerprinting of the volatiles present in these spore-forming plants, which can be used for identification and authentication of herbal samples, as well as for chemotaxonomic studies [2,3]. This lecture will cover the structures and biological activity of volatiles present in bryophytes, as well as chemotaxonomic studies. This lecture will also look at where bryophyte pharmacognosy may be directed in the future.

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# PL4. Linear retention index approach applied to liquid chromatography coupled to PDA and QqQ MS detectors for reliable characterization of oxygen heterocyclic compounds in essential oils and finished cosmetic products

Adriana Arigò[1,2], Paola Dugo[1,2], *Luigi Mondello*[1,2]*

*Keywords*: furocoumarins, cosmetics, LRI, HPLC-PDA, HPLC-MS/MS

Regulation (EC) n.1223/2009 of the European Parliament includes furocoumarins (FC) in the list of substances prohibited in cosmetic products except for normal content in natural essences used, the limit in sun protection and bronzing products is 1 mg/kg [1]. Despite the official regulations the *Scientific Committee on Consumers Products (ISCC)* and the *International Fragrance Association (IFRA)* are still proposing the maximum content of psoralens in rinse-off and leave-on products, according to the latest evidences of phototoxicity [2,3]. To date, LC coupled to PDA detector is the main technique employed for FC determination. However, the high Limits of Quantification (LOQs) suggested by IFRA, limit the HPLC-PDA application to the analysis of essential oils, making necessary the development of a more sensitive HPLC-MS method for the analysis of FC at trace level in the finished cosmetic products [4]. This work provides a detailed analysis of PDA LOQs calculated for several oxygen heterocyclic compounds, among FC, coumarins, and polymethoxyflavones. The linear retention index approach was used, for the first time, together with the UV library, as an extra criterion for the reliable characterization of the target compounds in the essential oils. The LRI of specific volatile compounds were calculated in order to identify the interfering compounds of the matrix which affect the LOQs. Calibration curves were created in pure solvent and by adding the standard compounds to different blank samples, with the aim to overcome the matrix effect. Moreover, LRI was applied to a new more sensitive HPLC-QqQ MS method, with MS and MS/MS (Multiple Reaction Monitoring) libraries and external calibration. The MS method was validated and used to determine the content of FC in cosmetics, such as perfumes and body wash.

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## PL5. Volatile compounds of the genus *Allium* L.

*Michael Keusgen*[1]*

*Keywords*: *Allium*, garlic, onion, wild onions, volatile sulphur compounds

*Allium* species like garlic (*A. sativum* L.), as well as common onion (*A. cepa* L.), are well investigated in terms of their sulphur compounds. In general, odorless cysteine sulphoxides like alliin or isoalliin will be converted by the enzyme alliinase into allicin and the so-called 'lachrymatory factor', respectively. These compounds are rather unstable and will form a huge variety of further volatile, characteristic smelling sulphur compounds. Moreover, more compounds have been discovered during the last years. Especially the mountainous areas of Middle and Southwest Asia are a rich source for wild-growing *Allium* plants. For instance, *A. tripedale* Trautv. belonging to the subgenus *Nectaroscordum* is naturally growing in the northwest of Iran and neighboring countries. Leaves have a very strong and hot taste and are widely used by the local population as a spicy vegetable. As a major constituent of the bulb, (+)-*S*-(1-butenyl)-L-cysteine sulphoxide ('homoisoalliin') could be identified. As volatile compounds, di-(1-butenyl)-disulphide and the cepaene-like compounds di-(1-*S*-sulphoxymethyl-butyl)-disulphide, 1-*S*-sulphoxymethyl-butyl-1'-*S*-sulphoxy-1-butenyl-butyl-disulphide and 1-*S*-sulphoxymethyl-butyl-1'-*S*-sulphoxybutyl-butyl-disulphide could be identified by various MS experiments [1]. Primary products resulting from the alliinase reaction of homoisoalliin seem to be highly unstable and were rapidly converted to the volatile compounds listed above. A further rather interesting species of this area is *A. stipitatum* Regel. Pyridinyl containing sulphoxides could be identified for the first time in the genus *Allium* [2]. It can be assumed that these compounds were converted into pyridinyl-*N*-oxides inside the plant. Corresponding *N*-oxides were also monitored after alliinase reaction giving the very typical odor of this species. Beside pyridinyl derivatives, the cysteine sulphoxide marasmin could be observed also yielding volatile sulphur compounds after alliinase reaction with at least three sulphur atoms. Especially *A. suworowii* Regel is rich in this compound delivering a unique smell and taste [3].

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# PL6. The regulatory framework for the quality and safe use of essential oils as herbal medicinal products. Selected examples from our Balkan "Neighbourhood"

*Ioanna Chinou*[1]*

*Keywords*: essential oils, regulatory, quality, safety, EU

All over the world medicinal plants and essential oils have been used therapeutically for centuries, and there are many conducted scientific studies that describe their remarkable healing properties. It is well known, that the chemistry of essential oils is influenced by the local geography, weather conditions, season and time of harvest, processing, packaging and storing conditions. The essential oils can be used mainly to be applied to the skin; to be inhaled; gargled and ingested, as well as bath additives. The methods of their administration result in absorption through the skin or oromucosa, and by inhalation.

The European Union has considered the medicinal use of essential oils as herbal products mainly through the Traditional Herbal Medicinal Products Directive (Directive 2004/24EC amending Directive 2001/83/EC as regards THMPs). The Herbal Medicinal Products Committee (HMPC) at the European Medicines Agency (EMA, London) has drafted and adopted guidelines which are intended to support assessment of THMPs considering their particular characteristics, while HMPC has established community monographs of herbal substances, and currently, about 13 monographs on essential oils (fennel, anise, peppermint, thyme, rosemary, lavender etc.), have been finalised and are available on EMA's website. In these monographs, the accepted quality, as well as the finally adopted indications among EU countries, together with potential risks, adverse reactions and contraindications in their uses, are presented, based in their longstanding medicinal uses and European experience. A viewpoint of the regulatory Authorities Experience in EU will be discussed, in detail, through Selected Examples mainly coming from our Balkan "Neighbourhood" (essential oils and other aromatic plants from the Balkan Peninsula).

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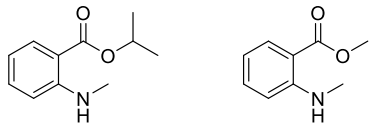
# PL7. Pharmacologically active derivatives of anthranilic acid occurring naturally in essential oils

*Fabio Boylan* [1]*

*Keywords*: methyl *N*-methylanthranilate, propyl *N*-methylanthranilate, isopropyl *N*-methylanthranilate, essential oil, pharmacological properties

Volatile anthranilic acid derivatives are important in the perfume industry since the second half of the 19th century. Methyl *N*-methylanthranilate (MMA) is the key component of neroli essential oil and it is present in other plants of the family Rutaceae. During the first decade of the 20th century, MMA was sold by several important perfume suppliers such as Schimmel, Van Dyk & Co, W.J. Blush & Co. but very little was known about its pharmacological/toxicological properties. Methyl (MMA) and isopropyl (IMA) esters of *N*-methylanthranilic acid have been recently identified in the essential oil of *Choisya ternata* Kunth (Rutaceae) (Fig. 1) [1]. Both of these volatile alkaloids have been proven to possess diverse pharmacological activities, including antinociceptive [1,2], anti-inflammatory [3], gastro-, hepato- and nephroprotective activities [4-6], anxiolytic and anti-depressant properties, as well as an effect on diazepam-induced sleep [7]. Although the toxicity of MMA has been previously investigated [2,8], there are only scarce data on the toxicity of IMA. In one of our previous studies [2], no signs of toxicity of IMA and MMA in mice (100 mg $kg^{-1}$, *p.o.*, 5-day study) were observed. Additionally, pathohistological examinations revealed no signs of liver toxicity or other signs of toxicity. When the metabolization studies were undertaken it could be concluded that generally, MMA and IMA suffer analogous biotransformation pathways; however, MMA predominantly underwent chemical conversions of the ester group, i.e. transformation into derivatives of anthranilamide and anthranilic acid, while the major metabolic pathway of IMA was hydroxylation of the aromatic core [9].




**1** **2**

Fig. 1. Isopropyl *N*-methylanthranilate (**1**) and methyl *N*-methylanthranilate (**2**)

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# INVITED SPEAKERS

| | | |
|---|---|---|
| **IS1** | *Yoshinori Asakawa* (Japan) | **Highly efficient production of functional substances from synthetic compounds and secondary metabolites by mammal and microbial biotransformation** |
| **IS2** | *Gordana Stojanović* (Serbia) | **Static headspace GC-MS analysis *versus* GC-MS analysis of essential oils** |
| **IS3** | *Neda Mimica-Dukić* (Serbia) | **Therapeutic efficiency of essential oils against *Helicobacter pylori* infections** |

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# IS1. Highly efficient production of functional substances from synthetic compounds and secondary metabolites by mammal and microbial biotransformation

*Yoshinori Asakawa*[1]*

*Keywords*: terpenoids, aromatic compounds, oxidation, *Aspergillus* sp., rabbits

We report herein a highly efficient production of several functional substances from synthetic aromatic compounds and plant secondary metabolites such as chalcones, mono- and sesquiterpenoids by microorganisms and rabbit. The microbial biotransformation was accomplished by four black fungi, *Aspergillus niger*, *A. sojae*, *A. usami* and *A. cellulosae* in rotatory growth cultures (120 rpm, Czapek-peptone medium at 30 °C for 3-10 days). In the case of biotransformation by mammals, each terpenoid and aromatic compound was orally administered to rabbits, and their collected urines were enzymatically treated to give each metabolite. *Aspergillus niger* cultured for 10 days in the presence of chalcone (**1**) (10 g / 200 mL medium) gave dihydrochalcone (**2**) in 95% isolated yield. The other *Aspergillus* strains converted chalcone to dihydrochalcone quantitatively. The substrate amount could be scaled up to 25 g / 200 mL medium. 4-Hydroxy- (**3**) and 4'-hydroxychalcones (**4**) incubated with the same *Aspergillus* afforded 4-hydroxydihydro- (**5**) and 3,4-dihydroxydihydrochalcones (**6**), and 4'-hydroxydihydro- (**7**) and 3',4'-dihydroxydihydrochalcone (**8**), in good yield, respectively. Thus, *Aspergillus* strains introduced a hydroxy group directly onto the already substituted benzene ring and very easily reduced the α,β-unsaturated double bond. 1,1-Diphenylmethane (**9**), 1,3-diphenylacetone (**10**), 1,3-diphenylpropane (**11**), bibenzyl (**12**), (*E* and *Z*)-stilbenes (**13, 14**) and phenylcyclohexane (**15**), grifolin (**16**), 6-shogaol (**17**), 6-gingerol (**18**), capsaicin (**19**), and dihydrocapsaicin (**20**) were also treated by *Aspergillus* strains to give the direct benzene ring hydroxylated products and ω-hydroxylation products, as well as epoxides, oxo- and hydroxyketo derivatives. (-)-α-Pinene (**21**) and β-caryophyllene (**22**) were converted by rabbits to *trans*-verbenol (**23**), an insect larvae pheromone, and 14-hydroxy-β-caryophyllene oxide (**24**), a constituent of mushrooms, in very high yield. Nootkatone (**25**), contributor to the grapefruit aroma, was obtained almost quantitatively from valencene (**26**), by a *Mucor* strain biotransformation. The metabolites of sesquiterpenoids, (+)- and (-)-cyclocolorenones (**27, 28**), (+)- and (-)-cuparenes (**29, 30**) and bisbibenzyls from liverworts, as well as the direct biotransformation of the corresponding essential oils are also reported. The presented methods are a cheap and hazard reduced eco-friendly alternative to classical organic synthesis while still reaching the high yields of the metabolites.

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## IS2. Static headspace GC-MS analysis *versus* GC-MS analysis of essential oils

*Gordana Stojanović*[1]*

*Keywords*: static headspace, essential oils, *Thymus*, *Peucedanum*, *Achillea*

The composition of essential oils (EO) of twelve plant species was compared with the corresponding headspace (HS) volatiles. Samples were prepared from fresh or dried whole above-ground parts, leaves, flowers and roots of the following plant species: *Achillea coarctata* [1], *A. crithmifolia* [2], *Angelica pancicii* [3], *Peucedanum longifolium* [4,5], *Chaerophyllum hirsutum* [6], *C. aureum* [7], *C. aromaticum* [8], *Origanum heracleoticum* [2], *Pastinaca hirsuta* [9], *Thymus glabrescens* [10], *T. praecox* [10], and *T. pulegoides* [10].

The following was noted:

- Monoterpenoids were present in HS volatiles with at least 90%.
- The investigated essential oils and the corresponding HS volatiles were different in quantitative terms for most monoterpenes while for the sesquiterpenes, there was an additional difference in qualitative terms.
- There was a negative correlation between the amount of thymol and carvacrol in EOs and the quantity of *p*-cymene and γ-terpinene in the HS.
- The same relationship was observed between linalool oxides and β-ocimenes.
- The relative amounts of α-terpineol, camphor and borneol were higher in the EOs when compared to HS volatiles.

From the above mentioned it can be concluded that HS analyses could not replace the analysis of EO but could be helpful in the cases when sufficient quantities of plant material are not available or when it is necessary to analyze a single specimen of a plant species.

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# IS3. Therapeutic efficiency of essential oils against *Helicobacter pylori* infections

*Neda Mimica-Dukić*[1]*, Nataša Simin[1], Dejan Orčić[1], Marija Lesjak[1], Petar Knežević[2], Verica Aleksić-Sabo[2], Krisztina Buzas[3]

*Keywords*: *Helicobacter pylori*, essential oils, linalool, thymol

*Helicobacter pylori*, a Gram-negative bacterium found in the stomach, is the cause of more than 90% of duodenal and 80% of gastric ulcers, and the major risk factor for gastric carcinoma and primary gastric lymphoma. Antibiotic therapy for treating *H. pylori* infections, the only available in current medical practice, has multiple disadvantages: lack of efficacy, development of resistance, adverse effects, and possible recurrence of the disease. Furthermore, the treatment is often associated with gastrointestinal side effects [1]. Consequently, there is a growing interest in the development of new antimicrobial therapeutic agents, more efficient against *H. pylori*, preferably of natural origin. Good candidates for that purpose are the volatile compounds present in essential oils. Due to the complexity of their composition, bacteria rarely develop resistance toward them [2]. Here, we reported the results of the efficacy of various essential oils, and their mixtures, against *H. pylori*. The highest *in vitro* activity was shown by *Satureja hortensis*, *Origanum vulgare* subsp. *vulgare* and *O. vulgare* subsp. *hirtum* essential oils. Furthermore, their binary and ternary mixtures exhibited notably higher antimicrobial activities [3]. The activity of the binary mixture of *S. hortensis* and *O. vulgare* subsp. *hirtum* essential oils (2MIX) was confirmed by an *in vivo* study in a mouse model, where changes in *H. pylori* colonization were detected by PCR and histological analyses of gastric samples. Furthermore, 2MIX show neither *in vitro* nor *in vivo* toxicity and do not have any immunomodulatory or allergic effect [4].

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# ORAL PRESENTATIONS

*Registration Fellowships founded by IFEAT and ISEO2018 Organizing Committee

| | | |
|---|---|---|
| **OP1** | *Petras Rimantas Venskutonis* (Lithuania) | **Essential oils from 11 *Cannabis sativa* cultivars isolated by different methods and toxicological evaluation of their components** |
| **OP2*** | *Margita Utczás* (Hungary) | **Novel analytical tool for a univocal flavor and fragrance identification: Gas chromatography coupled with condensed-phase FTIR and TOF mass spectrometry** |
| **OP3** | *Györgyi Horváth* (Hungary) | **Applicability of cinnamon bark essential oil in respiratory tract diseases–from *in vitro* to *in vivo* experiments** |
| **OP4*** | *Huong Thi Nguyen* (Hungary) | **Changes in the volatile compounds of two wormwood (*Artemisia absinthium* L.) accessions under controlled weather conditions** |
| **OP5*** | *Ewa Maciejczyk* (Poland) | **Juniper berry (*Juniperus communis* L.) supercritical extract, essential oil, and absolute comparison** |
| **OP6** | *Isiaka A. Ogunwande* (Nigeria) | **Chemical constituents, antiinflammatory and antinociceptive activities of essential oils from *Cordia millenii, Bougainvillea glabra* and *Phyllanthus muellerianus*** |
| **OP7** | *Guy Kamatou* (South Africa) | **An overview of the biological activities and essential-oil composition of three South African *Salvia* species** |
| **OP8*** | *Carmen M. S. Ambrosio* (Brazil) | **Chemical composition, antibacterial and antioxidant activities of a citrus essential oil and its fractions** |
| **OP9*** | *Ayaka Uehara* (France) | **Characterization of the odorant constituents of *Helichrysum italicum* essential oil** |
| **OP10*** | *Filomena Silva* (Spain) | **Cyclodextrin nanosponges as a new encapsulating agent for essential oils and their effectiveness against foodborne pathogens** |
| **OP11*** | *Milica Pejčić* (Serbia) | **Inhibitory effects of *Ocimum basilicum* and *Salvia officinalis* essential oils on virulence factors of *Pseudomonas aeruginosa* clinical isolates** |
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# OP1. Essential oils from 11 *Cannabis sativa* cultivars isolated by different methods and toxicological evaluation of their components

*Petras Rimantas Venskutonis*[1]*, Renata Baranauskienė[1], Orinta Aleknavičiūtė[1]

*Keywords*: *Cannabis sativa* cultivars, microwave assisted distillation, ultrasound assisted distillation, supercritical fluid extraction, essential oil composition

Industrial hemp is grown for numerous applications, traditionally for the production of textile fiber, pressing oil from the seeds and in foods. More recently, non-psychotropic phytocannabinoids have attracted an increasing interest of researchers and medics due to their health benefits. Industrial hemp accumulates comparatively low amounts of essential oil (EO); however, it is considered as an important ingredient for some hemp oil based products. The aim of this study was to expand the existing knowledge on the composition of EO compounds isolated from eleven *Cannabis sativa* cultivars using *Clevenger* hydrodistillation and supercritical $CO_2$ extraction (SFE-$CO_2$) for their isolation. In addition, microwave (MAD) and ultrasound (UAD) assisted distillation has been tested in order to evaluate their advantages. The dried plant material was ground using a 0.5-mm hole size sieve before EO isolation, while the fresh material was used undried. MAD was applied to the fresh material without its dilution with water, while SFE-$CO_2$ was performed in *Helix* extractor using 2 separators operating at different pressure and temperature. EO collecting vessel was cooled from –40 to +20 in order to evaluate possible losses of volatile constituents during system depressurization. The yield of EOs varied from 0.07 to 0.35% depending on the cultivar, extraction method, plant harvesting time, drying and SFE-$CO_2$ parameters. The main volatile components identified and quantified in *C. sativa* cultivars by GC×GC-TOF/MS and GC-FID, respectively, were β-caryophyllene (16.6-34%), humulene (13.1-30.0%), α-pinene (0.1-31.2%), caryophyllene oxide (4.3-10.2%), β-pinene (0.1-8.3%), myrcene (0.2-9.5%), limonene (0.1-2.7%), eucalyptol (0.1-3.1%), humulene epoxide II (1.4-3.6%) and *trans*-β-farnesene (1.3-4.6%). The toxicology of the main EO components was reviewed based on the previously reported data. In the second part of this study acetone extracts of the solid residue and water extracts consisting of the liquid phase after hydrodistillation were used for evaluating their antioxidant activities and total phenolic content in order to assess the possibility of using plant distillation residues as a source of various functional non-volatile ingredients. It was recently reported that the biorefining approach may give several valuable fractions from hemp threshing residues [1].

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# OP2. Novel analytical tool for a univocal flavor and fragrance identification: Gas chromatography coupled with condensed-phase FTIR and TOF mass spectrometry

*Margita Utczás*[1,2]*, Emanuela Trovato[2], Filippo Alibrando[2], Federica Vento[2], Luigi Mondello[2,3]

*Keywords*: flavor, fragrance, GC, TOF, FTIR

The correct identification of flavor and fragrance (F&F) compounds in real samples is still a challenge despite the huge number of different instruments available. Only a slight structural difference can cause a very different sensory profile, for example in the case of geometric isomers, it is generally considered that (*Z*)-isomers have a more pleasant and natural odor than (*E*) ones.

The most frequently used instrument for the analysis of volatiles is gas chromatography (GC) coupled with mass spectrometry (MS). MS may still fail to adequately identify compounds because of the lack of specificity of spectra (terpenes, isomers). MS spectral searches can be supported with linear retention index (LRI) information which, although not in all cases, could resolve the problem of possible misidentification of target molecules.

Condensed phase FTIR can be a complementary detection system to MS, and its application could allow a very detailed structural elucidation. The novelty of this instrument is that the separated compounds are condensed in small, singular spots on a rotating disc, thus the distortion of spectra is eliminated, giving an excellent spectral resolution. Through the specificity of the "fingerprint" region around 1100 $cm^{-1}$, even positional isomers and diastereomers could be distinguished.

Coupling condensed-phase FTIR after a simple post-column split to a GC-TOF MS, three independent analytical information can be obtained about the target compound: retention behavior (LRI), MS and FTIR spectra. Exploiting the enhanced resolution of the TOF MS and discriminating power of FTIR a unique TOF MS/FTIR spectral library with more than 1500 F&F compounds was developed, including also experimental LRI. Boosting this comprehensive information collection, a universal post-run software, namely CromatoPlus Spectra, performs the library search using the FTIR spectral similarity and LRI filter, simultaneously. A GC-TOF MS/FTIR method was optimized for the analysis of real essential-oil and perfume samples. Using the F&F library with embedded LRI, a reliable peak assignment was obtained for each separated compound.

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## OP3. Applicability of cinnamon bark essential oil in respiratory tract diseases–from *in vitro* to *in vivo* experiments

*Györgyi Horváth*[1]*, Kamilla Ács[1], Viktória L. Balázs[1], Eszter Csikós[1], Ashraf Amir Reza[1], Béla Kocsis[2], Andrea Böszörményi[3], Barbara Horváth[4], Aleksandar Széchenyi[4], László Kereskai[5], Kata Csekő[6], Ágnes Kemény[6], Zsuzsanna Helyes[6,7]

*Keywords*: cinnamon oil, vapor phase, biofilm, respiratory tract, inflammation

*Introduction*: Because respiratory tract diseases affect every age group and antibiotic resistance is an increasing problem in healthcare, there is a need for additional therapies. Essential oils (EOs) are used via inhalation for the treatment of respiratory tract diseases for a long time. Similarly to other plant extracts, their efficacy should also be proved in several test systems. Therefore, our aim was to study the antibacterial and antiinflammatory effects of cinnamon bark oil in *in vitro* and *in vivo* models.

*Methods*: The chemical composition of cinnamon EO was determined by GC-FID/MS and SPME-GC-MS methods. The antibacterial effect of the EO was tested by macrodilution and vapor-phase methods against respiratory tract pathogens. The emulsion of the EO prepared by nanotechnology was also used for the examination of the biofilm inhibitory effect. The antiinflammatory effect was studied in an LPS-induced acute airway inflammation mouse model.

*Results and conclusion*: The main component of the EO was *trans*-cinnamaldehyde (74.0%, 46.0%) in both analytical systems. In the liquid medium, cinnamon EO exhibited antibacterial activity against *Streptococcus pyogenes*, *S. pneumoniae*, *S. mutans*, *Haemophilus influenzae* and *H. parainfluenzae* (MIC: 0.06 mg/mL). In the vapor-phase test, the EO was the most effective against *Haemophilus* strains (MIC: 15.6 µL/L). The biofilm formation of *S. mutans* was more effectively reduced by the emulsion of cinnamon oil prepared by nanotechnology compared to the emulsions prepared with Tween80 or alcohol. In the animal model, cinnamon oil inhalation reduced airway hyperreactivity, macrophage accumulation in histological images, but did not affect MPO activity. Therefore, cinnamon oil may be a potential antibacterial and antiinflammatory agent for the treatment of respiratory tract diseases.

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# OP4. Changes in the volatile compounds of two wormwood (*Artemisia absinthium* L.) accessions under controlled weather conditions

*Huong Thi Nguyen*[1]*, Éva Zámboriné-Németh[1]

*Keywords*: environment, *cis*-epoxyocimene, sabinene, essential oil, temperature

Two wormwood accessions (originating from Spain and Hungary) were grown in climatic chambers in order to determine the effect of temperature and light intensity on the composition of their volatile compounds. Young plants were grown in a controlled environment termed as "warm" (increasing temperature from 18 °C/10 °C to 27 °C/19 °C and 16 klx light intensity with a 14 h/10 h light-dark rhythm, respectively) and "cold" ones (increasing temperature from 13 °C/8 °C to 18 °C/ 10 °C and 8 klx light intensity with a 14 h/10 h light-dark rhythm, respectively) for 14 weeks.

The EO yield of the investigated accessions varied from 0.188 mL/100 g ("Hungarian" accession grown in the "warm" chamber) to 1.092 mL/100 g ("Spanish" accession grown in the "cold" chamber) and the installed weather programs had no effect on the EO yield of any of the accessions. Evaluating the components higher than 1% of all detected GC areas, 33 compounds were identified with the total identified percentage varying from 88.8% ("cold" treatment of the "Hungarian" accession) to 92.5% ("cold" treatment of the "Spanish" accession). The well-established chemical differences between the two investigated accessions of wormwood, determined in our former study [1], have been confirmed by the present data. The major components of the oils were sabinene (0-10.8%), β-myrcene (1.7-16.5%), *cis*-epoxyocimene (1.2-57.7%), *cis*-chrysanthenyl acetate (0-13.8%), and (*Z*)-nuciferyl isobutyrate (1.7-10%). The "Spanish" accession represents a "*cis*-epoxyocimene" chemotype while the "Hungarian" accession exhibits a much more variable profile with sabinene and β-myrcene as the most characteristic components. The results showed that the accumulation of volatile compounds was not influenced by the weather under the investigated parameters. However, the different weather conditions induced quantitative changes in the EO profile of both chemotypes. The relative amount of *cis*-chrysanthenyl acetate increased from 8.0 ("cold" chamber) to 13.8% ("warm" chamber) in the oil of the "Spanish" plants while sabinene increased from 2.3 to 10.8% and β-myrcene rose from 8.0 to 16.5% in the "cold" and "warm" chambers, respectively, for the "Hungarian" oil samples.

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# OP5. Juniper berry (*Juniperus communis* L.) supercritical extract, essential oil, and absolute comparison

*Ewa Maciejczyk*[1]*, Magdalena Kuśmierz[1], Agnieszka Dębczak[2], Edward Rój[2], Danuta Kalemba[1]

*Keywords*: *Juniperus communis* supercritical extract, juniper berry essential oil, concrete, absolute

Supercritical fluid extraction (SFE) of essential-oil constituents has absorbed much attention, especially in cosmetic, pharmaceutical and food industries, because it is an alternative to conventional processes such as organic-solvent extraction and steam distillation [1]. SFE of plant material with $CO_2$ allows its processing at low temperatures, therefore limiting the thermal degradation of its components, and avoiding the use of solvents prohibited in cosmetic or food products [1]. Moreover, it was shown that essential-oil constituents and light fractions of the resins are selectively extracted with this technique, producing an extract with the characteristics of the absolute [2].

Juniper berries, *Juniperus communis* L. (Cupressaceae), are a rich source of both volatile terpenes and lipophilic compounds with higher molar masses, such as resins and fats. The analysis of juniper berry supercritical extraction processes indicated unequivocally that, depending on the chosen process parameters, it is possible to obtain extracts from the same raw material in a different yield, with different chemical composition, physical and organoleptic properties.

The compositions of the essential oil (EO), absolute and supercritical $CO_2$ extract of juniper berries were analyzed by GC–MS. The chemical composition and physical properties of the extract run at 80 bar and temperature of 40 °C were similar to the juniper berry essential oil. However, it showed a lower ratio of terpene hydrocarbons to their oxygenated derivatives in comparison with the EO, which is reflected in its smell: more beneficial and natural–similar to the absolute odor.

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# OP6. Chemical constituents, antiinflammatory and antinociceptive activities of essential oils from *Cordia millenii, Bougainvillea glabra* and *Phyllanthus muellerianus*

Opeyemi N. Avoseh[1], Oladipupo A. Lawal[1], Olawumi P. Afolabi[1], Kazeem N. Olasunkanmi[1], Daniel O. Igile[1], *Isiaka A. Ogunwande*[1]*, Roberta Ascrizzi[1,2], Flamini Guido[2]

*Keywords*: *Cordia millenii, Bougainvillea glabra, Phyllanthus muellerianus,* antiinflammatory activity, antinociceptive activity

Essential oils were obtained by hydrodistillation of air-dry leaves of *Cordia millenii* Bak. (Boraginaceae), *Bougainvillea glabra* Choisy (Nyctaginaceae) and *Phyllanthus muellerianus* (Kuntze) Exell. (Euphorbiaceae) using a Clevenger-type apparatus. The chemical constituents of the oils were analyzed by gas chromatography and gas chromatography-mass spectrometry on an HP-5MS column. The major constituents of *C. millenii* were limonene (19.9%), diallyl disulfide (18.4%), β-caryophyllene (16.6%) and linalool (13.4%) while (*E*)-nerolidol (31.4%), (*E*)-β-ionone (10.3%) and linalool (10.1%) were present in *B. glabra*. Hexahydrofarnesyl acetone (11.6%), isocaryophyllene (9.8%) and limonene (9.4%) occurred in higher proportions in *P. muellerianus.* The antinociceptive properties of *C. millenii* oil were statistically not significantly different ($p>0.05$) when compared to the control for most tested concentrations except at the 120$^{th}$ minute ($p<0.05$) for the dose of 200 mg/kg *p.o*. This dose displayed antiinflammatory activity only at the 1$^{st}$ hour ($p<0.01$) while the others were statistically not significantly different ($p>0.05$) when compared to the control. The antinociceptive properties of the essential oil of *B. glabra* were statistically significantly different, $p<0.05$ and $p<0.01$ at the doses of 100 and 200 mg/kg *p.o*., respectively, when compared to the control at the 30$^{th}$ minute but much more effective ($p <0.001$) at a dose of 400 mg/kg. For the 1$^{st}$ and 2$^{nd}$ hour, at the doses of 100 and 200 mg/kg ($p <0.001$), the antiinflammatory activity was statistically significantly (very low values of *p*) different from the control, while at the 3$^{rd}$ hour, it was significant ($p <0.01$) at a dose of 300 mg/kg but there were no statistical differences observable at the 4$^{th}$ hour. The essential of *P. muellerianus* at 100 mg/kg *p.o*. displayed an increased antinociceptive activity with $p<0.01$ to $p <0.001$ from the 30$^{th}$ to the 120$^{th}$ minute. Moreover, the oil showed a high inhibition, with up to $p <0.001$, in the case of carrageenan-induced inflammation.

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## OP7. An overview of the biological activities and essential-oil composition of three South African *Salvia* species

*Guy Kamatou*[1]*, Maxleene Sandasi[1], Alvaro Viljoen[1,2]

*Keywords*: *Salvia*, biological activities, bisabolol, ethnobotany

Essential oils produced by aromatic plants have been used to treat various ailments such as malaria and microbial infections for many years. In South Africa, there are 26 indigenous *Salvia* species and most of them have been reported for use in the treatment of malaria, tumors, microbial infections. Among those of ethnomedicinal value are *S. repens*, *S. stenophylla* and *S. runcinata* which form a species complex. The current study aimed to profile the essential-oil composition and investigate the bioactivities related to the traditional uses. The essential oil of the three species (*S. repens*, *S. stenophylla* and *S. runcinata*) was isolated by hydrodistillation and the antimalarial, anti-inflammatory, antimicrobial activities and the toxicity profiles were evaluated using the [$^3$H]hypoxanthine incorporation assay, 5-lipoxygenase assay, minimum inhibitory concentration assay and the MTT colorimetric method, respectively. The essential-oil composition was analyzed using the GC-MS and GC-FID methods. The oil of *S. repens* was dominated by 1,8-cineole (12.8%), *p*-cymene (9.5%) and limonene (9.4%), while α-bisabolol (65.0%) and β-caryophyllene (10.5%) were the major constituents of *S. runcinata*. α-Bisabolol (26.1%) and δ-3-carene (22.6%) were the dominant constituents of *S. stenophylla*. The anti-inflammatory activity of the three oils ($IC_{50}$ value) ranged from 22.8 to 49 µg/mL with *S. runcinata* exhibiting the best activity. The three oils also inhibited the growth of *Plasmodium falciparum* FCR-3 strain with $IC_{50}$ values ranging from 1.2-4.1 µg/mL with the oil of *S. runcinata* showing the best antimalarial activity. The essential oils showed poor antimicrobial activity (MIC value > 32 mg/mL) and were also toxic to normal kidney epithelial cells ($IC_{50}$ value < 6.6 µg/mL). The essential oils displayed some degree of activity, however, the toxicity exhibited against kidney cells indicated that the oils should be used with caution.

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# OP8. Chemical composition, antibacterial and antioxidant activities of a citrus essential oil and its fractions

*Carmen M. S. Ambrosio*[1]*, Elena Stashenko[2], Carmen J. Contreras Castillo[1], Eduardo M. Da Gloria[1]*

*Keywords*: fractional distillation, limonene, *E. coli*, *Lactobacillus*

The prohibition of antibiotic use in animal feed since 2006 by the European Community, due to the concern about the growing emergence of bacterial resistance, has led to the search for alternatives to substitute antibiotics. Essential oils (EOs) could be a possible alternative because of their antimicrobial properties. Specifically, citrus EOs, that are by-products of orange juice production, could be an excellent alternative since they have shown a good potential to fight pathogenic bacteria and their use in animal feed could become feasible since there is a high availability of them in the worldwide market. The aims of this study were to evaluate the chemical composition, antibacterial and antioxidant activities of a commercial citrus EO, Brazilian orange terpenes (BOT), and its fractions. Initially, the antibacterial activity of BOT was tested on *Escherichia coli* U21 (K88 LT/STb/F18/STa) isolated from pig gut and on *Lactobacillus rhamnosus* ATCC 7469 by a microdilution method. MIC and MBC results showed that *E. coli* (MIC=MBC=1.85 mg/mL) was more sensitive than *L. rhamnosus* (MIC=3.7 and MBC=7.4 mg/mL) to BOT, thus it displayed a selective antibacterial activity, affecting more the pathogenic than the beneficial bacteria. Limonene (78.7%) was determined as the major compound in BOT by GC-MS. After that, BOT was subjected to fractional distillation in a pilot system of continuous distillation. Four fractions were obtained: F1, F2, F3, and F4. The first three fractions were characterized by a high relative amount of limonene (86.9; 91.8; 91.9%,) followed by *cis*-limonene oxide, *trans*-limonene-oxide, and myrcene. Conversely, F4 was characterized by having the lowest amount of limonene (0.96%) and as having *trans*-carveol, carvone, *cis-p*-mentha-2,8-dien-1-ol, and *trans-p*-mentha-2,8-dien-1-ol as the major compounds. Only F4 was demonstrated to have an activity on *E. coli* (MIC=MBC=3.7 mg/mL) and *L. rhamnosus* (MIC=MBC=14.8 mg/mL). The F4 fraction also possessed the highest antioxidant activity (845.7 $\mu mol_{trolox}/g$ - ORAC) in contrast to the others fractions (479.7; 334.4; 209.1 $\mu mol_{trolox}/g$, respectively), and even to the EO itself (785.1 $\mu mol_{trolox}/g$). The results imply that the minor compounds were responsible for the biological activity of this EO instead of its major compound limonene.

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## OP9. Characterization of the odorant constituents of *Helichrysum italicum* essential oil

*Ayaka Uehara*[1], Stéphane Andreani[1], Niko Radulović[2], Nicolas Baldovini[1]*

*Keywords*: *Helichrysum italicum* subsp. *italicum* (Asteraceae), curry plant, GC-O, aroma extract dilution analysis (AEDA)

*Helichrysum italicum* ssp. *italicum* (Asteraceae) is widespread all over the Mediterranean basin. It is sometimes called the "curry plant" because of the typical strong spicy smell of its leaves. In the flavor & fragrance industry, this species is extracted for the production of the absolute, or hydrodistilled to furnish an essential oil which is widely used in cosmetics and in aromatherapy. The composition of the essential oil has been extensively studied, and depending on the geographical origin of the plant, the main constituent is either neryl acetate **1** or monoterpenes like α-pinene **2** (Fig. 1). Some uncommon 2-methyl-1,3-diketones such as **7**-**11** appear to be specific components of *H. italicum* and have never been observed in other species so far [1,2]. In the course of our analytical studies devoted to the identification of the key odorants of fragrant plants, we performed a Gas Chromatography-Olfactometry (GC-O) analysis of a sample of Corsican *H. italicum* essential oil (neryl acetate type), using the Aroma Extract Dilution Analysis (AEDA) methodology. The identification of the odorants was realized by a detailed fractionation of the essential oil by liquid-liquid basic extraction, distillation and column chromatography, followed by GC-MS and GC-O analyses of some fractions, and co-injection of commercial and synthesized reference compounds. We could demonstrate that the characteristic curry/spicy odor of the plant was mostly due to the saturated diketones **7** and **8**, together with some other volatiles more common as essential-oil constituents (such as 1,8-cineole **3**, nerol **4**, eugenol **5**, *p*-cresol **6**, etc.). In contrast, the olfactory contribution of **1** and of the unsaturated diketones **9**, **10** and **11** was much less significant.

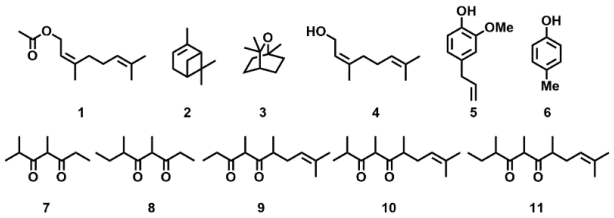


Fig. 1. Main constituents and odorants of *Helichrysum italicum* essential oil.

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# OP10. Cyclodextrin nanosponges as a new encapsulating agent for essential oils and their effectiveness against foodborne pathogens

*Filomena Silva*[1,2,3]*, Ilaria Simionato[2], Celia Domeño[3], Fernanda C. Domingues[4], Cristina Nerín[5]

*Keywords*: cyclodextrin nanosponges, cinnamon essential oil, coriander essential oil, antimicrobial activity, foodborne pathogens

In this work, we exploit the antimicrobial properties of cinnamon and coriander [1] essential oils that are incorporated in cyclodextrin nanosponges to create a stable controlled release system for these oils. For this purpose, cyclodextrin (CD) nanosponges (NS) were loaded with coriander (COO) and cinnamon essential oils (CIO) and evaluated for their antimicrobial activity against common foodborne pathogens both in direct contact as well as in vapour phase. To evaluate the loading capacity of the nanosponges, two SPME-GC-MS methods were successfully validated for the major compounds present in COO and CIO. The results demonstrated that loading was dependent on the type of solvent used and that nanosponges have different affinities for the oils tested as well as for each of their components. The results showed that, for COO, the NS with higher loading capacity were the ones based on β- and HP-β-CD; while for CIO, α- and β-NS were the ones yielding the best encapsulation efficiencies. The results showed that COO and CIO loaded nanosponges can effectively release essential oils and are able to exert their antimicrobial activity both in liquid medium as well as in the vapour phase. Overall, these results suggest that these nanosponges can effectively load and release COO and CIO to exert their antimicrobial activity, which opens the doors for their potential use in antimicrobial food packaging applications.

*References*:
[1] Silva, F., Domingues, F.C., 2017. Crit. Rev. Food Sci. 57, 35–47.

*Acknowledgments*: This work was partially funded by Fundação para a Ciência e Tecnologia through a fellowship (SFRH/BPD/79250/2011) and a project (PEst-C/SAU/UI0709/2011). The authors also acknowledge the funding provided by the Gobierno de Aragón (Spain) and Fondo Social Europeo to the GUIA group (financiación grupo GUIA T-10).

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# OP11. Inhibitory effects of *Ocimum basilicum* and *Salvia officinalis* essential oils on virulence factors of *Pseudomonas aeruginosa* clinical isolates

Zorica Stojanović-Radić[1]*, *Milica Pejčić*[1], Marina Dimitrijević[1], Nikola Stanković[1], Marija Genčić[2], Niko Radulović[2]

*Keywords:* pyocyanin, motility, clinical isolate, essential oil, virulence

*Pseudomonas aeruginosa* is a Gram-negative human opportunistic pathogen, responsible for a variety of human health disorders. The virulence of each *P. aeruginosa* strain is strongly related to its capability of biofilm formation, different types of motility, production of toxins and pigments. Essential oils of basil and sage have a wide range of applications in the traditional and/or official medicine. The aim of the present study was to evaluate the activity of basil (*Ocimum basilicum*) and sage (*Salvia officinalis*) commercially available essential oils on *P. aeruginosa* virulence factors (post-adherence biofilm production, resistance of a mature biofilm, motility and production of pyocyanin). Antipseudomonal efficacy was studied using the microdilution method and the obtained minimal inhibitory concentrations (MICs) were further used to explore the anti-virulence potential. The experiments were performed against a panel of *P. aeruginosa* clinical isolates of different origin at 1/2 x MIC, MIC, and 2 x MIC concentrations.

The two essential oils were chemically characterized by GC and GS/MS analyses, where linalool and (*E*)-anethole where found to be the dominant compounds in the basil oil sample, while α-thujone and camphor were the major constituents of the sage essential oil sample. The biofilm experiments demonstrated a very high activity of both oils to biofilm production, where basil oil showed a higher efficiency by inhibiting up to 92.7% of the biofilm produced by the control, while sage oil exhibited a reduction of 9.8 to 76.8%. Promising results were also obtained when the oils were applied to mature biofilms, where reductions of 2.4-84.1% and 13.8-75.8% were measured for basil and sage oils, respectively. The results on motility evaluation showed that, in the presence of both oils, swimming, swarming and twitching motility patterns were significantly affected. Experiments on the pyocyanin production showed a reduction from 20.7-60.9% and 5.0-60.5% caused by the basil and sage oils, respectively.

Considering all the obtained results, it can be concluded that both basil and sage essential oils present highly efficient antipseudomonal agents which could be used against infections caused by this pathogen.

*Acknowledgments*: The work was funded by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Project No. 172061).

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## OP12. Evidences for lemon-balm essential oil suppression of anxiety-related behavior in animal and *in vitro* models

*Nikola M. Stojanović*[1]*, Pavle Randjelović[1], Marko Mladenović[2], Nenad Stojiljković[1], Sonja Ilić[1], Gordana Nikolić[1], Niko S. Radulović[2]

*Keywords*: *Melissa officinalis*, anxiety, skeletal muscle tonus, gastrointestinal motility, acetylcholinesterase

Anxiety disorders are among the most frequent psychiatric diseases, with around ¼ of the World population suffering from these disorders during their lifetimes. Besides psyche-related symptoms, these patients can have a large number of somatic symptoms as well. Although the treatment of these disorders is mainly focused on resolving its mental component, one cannot neglect the need for the treatment of accompanying somatic symptoms. *Melissa officinalis* L. (lemon balm), in various formulations, has been extensively used as an ethnomedicinal remedy for the treatment of different psyche-related symptoms and its use is considered relatively safe. In the present study, the potential activity of *M. officinalis* essential oil was evaluated in several *in vitro* models and *in vivo* animal studies mimicking or involving anxiety-related somatic symptoms. Effects of *M. officinalis* essential oil on BALB/c mice motor activity was estimated using an open field, rotarod and horizontal wire tests. The performance of mice treated with 25 mg/kg of the oil showed a statistically significant decrease in the motor impairment arising from acute anxiety (open field test), while there was a prolonged latency and a reduction of the frequency of falling from a rotating rod and/or a horizontal wire (signs of muscle weakness/spasms). Additionally, the essential oil was assayed for its potential in inhibiting acetylcholinesterase activity and was found to be a very weak enzyme inhibitor. The potential beneficial properties of the essential oil on the function of the gastrointestinal system were evaluated in the models of spontaneous and induced isolated mouse ileum contractions. Concentrations of the essential oil higher than 1 μg/mL were found to inhibit both spontaneous and induced ileum contractions. The observed activity of the essential oil could be attributed to a large number of different constituents of the oil, most probably the monoterpenes which represent more than 50% of the oil.

*Acknowledgments*: This work was supported by the Ministry of Education, Science and Technological Development of Serbia [Project No. 172061].

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## OP13. Cytotoxicity and the effect on the inflammation response of thyme oil and thymol: evaluation in human macrophage cells

*Leidy Jaqueline Angel Ferro*[1], Sophie Iglewski[2], Péter Bukovics[2], Kitti Garai[1], Krisztina Bánfai[1], Béla Kocsis[3], Andrea Böszörményi[4], Krisztián Kvell[1], Györgyi Horváth[2]*

*Keywords*: Thyme oil, LPS, TNFα, flow-cytometry, qPCR

The essential oil of *Thymus vulgaris* L. (Lamiaceae), thyme oil, shows a great variability of its composition with six main chemotypes recognized up to now: geraniol, linalool, γ-terpineol, carvacrol, thymol, and *trans*-thujan-4-ol/terpinen-4-ol types. Due to this large chemical diversity, the subject of several investigations was to identify and determine their properties, including their potential effect on inflammation. In our previous microbiological study, this essential oil showed a significant antibacterial activity against bacteria of the respiratory tract [1].

The present research focuses on the evaluation of its cytotoxic and antiinflammatory effect in the case of the U937 human monocyte/macrophage cell line. Thyme oil composition was determined by GC/MS. Bürker chamber was used for cell counting and flow-cytometry to evaluate cellular toxicity (using 7-AAD). Then a qPCR method was used to determine the expression of TNFα mRNA.

The main component of the tested sample of thyme oil was thymol (38.7%) that showed a concentration-dependent cytotoxicity. Non-toxic dilutions showed preventive antiinflammatory potential.

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*Acknowledgments*: The project has been supported by the European Union, co-financed by the European Social Fund (EFOP-3.6.1.-16-2016-00004) and Faculty of Medicine, University of Pécs (PTE ÁOK-KA No: KA-2018-01).

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## OP14. The Jerusalem Balsam–a case study of a 150-year-old sample

*Jacek Łyczko*[1]*, Aleksandra Pawlak[2], Antoni Szumny[1], Marcelin Petryja[3], Henryk Różański[4]

*Keywords*: cytotoxicity, essential oils, Jerusalem balsam

The Jerusalem Balsam (JB) was formulated in the pharmacy of the Saint Savior monastery in the old city of Jerusalem in 1719. According to traditional sources, JB was based on an ethanolic extract of an herbal mixture. Several variations of the formulation could be found in European Pharmacopoeias, mostly recommended as an antiseptic product [1]. During the current study, an original sample of JB prepared approximately in the year 1870, as well as four contemporary samples of different variations in composition, were analyzed by gas chromatography coupled with mass spectrometry with the aid of solid phase microextraction, as well as by the liquid injection approach. About sixty different compounds have been identified in the materials–mostly essential-oil constituents. Additionally, the LC-MS and NMR ($^1$H, HSQC, and TOCSY) profiles have been measured for the analyzed samples. Several fingerprint compounds, specific for the herbal material were found in this way. Furthermore, JB samples were tested for cytotoxicity. Two normal (J774E.1 and NIH/3T3) and two cancer cell lines (CLBL-1 [2] and CLBL70 [3]) were used in this experiment. All tested JB samples showed no cytotoxic or were very slightly toxic to normal cell lines. Only one JB sample, the almost 150-year-old one, showed a strong cytotoxic activity but only towards cancer cell lines, with the efficiency of 80-90%.

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[1] Barana, H. et al., 2017. J. Tradit. Med. Clin. Natur. 6, 224.
[2] Rütgen, B.C. et al., 2010. Leukemia Res. 34, 932–938.
[3] Pawlak, A. et al., 2017. Vet. Comp. Oncol. 15, 1218–1231.

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## OP15. Microemulsions of essential oils–an improvement of solubility or something more?

*Elwira Sieniawska*[1]*, Michał Wota[1], Tomasz Mroczek[1]

*Keywords*: microemulsions, essential oils, activity, solubility

The direct application of essential oils in an aqueous solution is significantly hampered by the limited solubility in the aqueous environment and the volatile nature of these mixtures. Colloidal systems in the form of microemulsions and nanoemulsions [1] can effectively disperse essential oils in water, what is needed in many biological tests and applications.

The aim of this work was to prepare stable, water-dilutable, microemulsions containing essential oils of citronella (*Cymbopogon nardus*), mint (*Mentha x piperita* 'Multimentha') and eucalyptus (*Eucalyptus globulus*) essential oils (EO) and the mixture of their equal parts. The possible antioxidant and antimicrobial applications of the obtained formulations were tested.

Nine runs were made in which the aqueous phase, being a mixture of water and polypropylene glycol in a 1:1 volume ratio, ranged from 10 to 90%, v/v. The oily phase was a mixture of the essential oil and soybean oil in a volume ratio of 3:1. Polysorbate 80 with an oil phase in 5 different volume ratios varying from 5:1 to 9:1 was mixed in each series. The essential oils constituted from 0.8 to 11% of the microemulsions. The diameter of the obtained microemulsion droplets was measured using the direct light scattering technique.

Stable microemulsions were obtained in the range between 10 and 50% of the aqueous phase. They were fully dilutable with water. The measurement of the diameter of the droplets for the formulations comprising 50% of the aqueous phase and diluted 10 times with water showed that particles of the oil dispersed in water were in the range between 10 and 20 nm. The formulations showed an increase in the antioxidant activity compared to the controls, whereas their antimicrobial activity was not influenced.

*References*:
[1] McClements, D.J., 2012. Soft Matter 8, 1719–1729.

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# SPONSOR PRESENTATIONS

| | | |
|---|---|---|
| **SP1** | *Neža Rangus* (ARXFARM d.o.o., Slovenia) | ***Helichrysum* oil from the Balkan peninsula** |
| **SP2** | *Nikunj R. Harlalka* (SANKHUBABA INTERNATIONAL, India) | **Community-based production and organic certification of aromatic & medicinal crops in India** |

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# SP1. *Helichrysum* oil from the Balkan Peninsula

*Neža Rangus*[1]*

*Keywords*: *Helichrysum* oil, essential oils, Balkan Peninsula

*Helichrysum italicum* (Roth) G.Don (Asteraceae) is widespread in the Mediterranean area and represented by several subspecies. Among them *Helichrysum italicum* (Roth) G.Don subsp. *italicum* is the main source of commercial *Helichrysum* oil, used in aromatherapy and natural cosmetics due to antiaging properties.

In the recent time, a big cultivation area was established along the Adriatic coastal region, where the plant is native, and the continental area including Bosnia and Hercegovina, Serbia, Greece, and Bulgaria.

The chemical composition of *Helichrysum* oil can vary and depends on the subspecies and habitat. The main constituents are: monoterpenes (α- and β-pinenes, limonene), monoterpenes esters (neryl acetate), sesquiterpenes (italicene, α-humulene, β-caryophyllene, α-copaene, α-, β- and γ-curcumenes, α- and β-selinene) and diketones (italdiones).

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# SP2. Community-based production and organic certification of aromatic & medicinal crops in India

*Nikunj Ramakant Harlalka*[1]*

*Keywords*: organic certification, national horticulture mission, Wadi project

*India has been one of the leading producers of essential oils for Industrial applications. The journey first began from Lemongrass Oil in 19th Century to Menthol and Mint-based derivatives in recent years. As the consumer is demanding more traceability, community-based projects in the country are reaching out for organic certification and fair trade carving a niche for them. The article covers the journey of these marginalized communities and the ways in which they are keeping up with the changing consumer preferences and regulatory requirements.*

Essential-oil production from perennial aromatic crops became a challenge after the green revolution which laid emphasis on food production. Once India's food production targets were met in 2002, the government launched the National Horticulture Mission. This mission aimed at increasing the production of horticulture products. Since fruit trees had a gestation time of 4-5 years, the aromatics crops became the preferred choice. Intercropping aromatic crops in fruit orchards thus gained popularity. On similar lines, 'Wadi Project' gained momentum in the 90's. India's tribal population is concentrated in the Central region comprising the States of Chhattisgarh, Jharkhand and Orissa. These states, being sparsely populated and economically backward, provided an ambient environment for the development of essential oils.

More recently these communities have been going organic by getting their clusters certified. As India had National standards for Organic Production and equivalence agreements with EU their produce found seamless access to the global markets. In 2013 when the import authorization system threatened to jeopardize exports of certified organic products from India, it was their combined strength which found back and restored the trade. Alongside essential oils, this region has been an important source of medicinal herbs for the Ayurvedic Industry and joint forest management programs have been in place for the collection of wild herbs for over 20 years. These 'van-samiti' (Translates Van=Forest, Samiti= Committee) which consists of members of the rural community and forest authorities serve as just the right kind of network for sustainable collection of medicinal herbs in the wild. At present, over 50 community-based projects spread across 3000 hectares are engaged in essential-oil production. The strength of these projects lies in the use of spent biomass to fuel distillation units. These projects are backed by Government programs and implemented by non-governmental organizations along with marketing tie-up with the Industry.

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# WORKSHOP

*Registration Fellowships founded by IFEAT and ISEO2018 Organizing Committee

| | | |
|---|---|---|
| **WS*** | *Dragan Zlatković* (Serbia) | **GC-MS made easy: AMDIS in the analysis of complex mixtures of volatiles** |

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# WS. GC-MS made easy: AMDIS in the analysis of complex mixtures of volatiles

Dragan Zlatković[1]*

*Keywords*: GC-MS, AMDIS, essential-oil analysis

The Automated Mass Spectral Deconvolution and Identification System (AMDIS) is a computer program that extracts pure component spectra from complex chromatograms and identifies target compounds by matching these spectra against a reference library [1,2]. This software is a powerful tool that can be used as a "black box" device to identify trace compounds in complex matrices, yet it is available free of charge from the webpage of the National Institute of Standards and Technology (NIST) [3]. The workshop will cover basic operations and tools available in AMDIS (including chromatogram manipulation, retention index calculation, peak integration and library search), as well as more advanced concepts and methods that can be useful to an essential-oil chemist. The workshop is intended primarily for PhD students and researchers new to the analysis of complex volatile mixtures. It is desirable that participants have a basic knowledge of GC-MS principles.

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[1] Davies, T., 1998. Spectrosc. Eur. 10, 24–27.
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# POSTER PRESENTATIONS

**Poster sessions:**

*Session I*: Odd numbers (like PP1, PP3, etc.) – Friday, September 14
*Session II*: Even numbers (like PP2, PP4, etc.) – Saturday, September 15

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| **PP1** | *Tadaaki Satou* (Japan) | **The influence of two Lamiaceae essential oils on dementia-related symptoms in animal models** |
| **PP2*** | *Margita Utczás* (Hungary) | **Cannabis terpene profiling in therapeutic products by means of gas chromatography coupled with mass spectrometry** |
| **PP3*** | *Filomena Silva* (Spain) | **The use of essential oils for antimicrobial food packaging** |
| **PP4** | *Eleni Stavraki* (Greece) | **Chemical analyses of truffle flavored (*Tuber* spp.) olive oils on the Greek market with HS-SPME** |
| **PP5** | *Ana Dobreva* (Bulgaria) | **On the subcritical extraction of *Rosa damascena* Mill.** |
| **PP6** | *Ana Dobreva* (Bulgaria) | **The impact of soil herbicides on the yield and quality of lavender (*Lavandula angustifolia* Mill.) essential oil** |
| **PP7** | *Alexandra Machado* (Portugal) | **Volatiles characterization of different commercial honey types from the Azores (Portugal)** |
| **PP8** | *Jelena Aksić* (Serbia) | **New neryl esters from *Helichrysum italicum* essential oil** |
| **PP9** | *Jelena Aksić* (Serbia) | **Antimicrobial and anti-inflammatory potential of different immortelle essential-oil chemotypes** |
| **PP10** | *Suzan Kelly Bertolucci* (Brazil) | **Effect of macro- and micro-element-deficiency on growth and essential-oil composition of *Mentha arvensis L.* cultivated in solution** |
| **PP11** | *Paulo R. Moreno* (Brazil) | **Chemical composition and antimicrobial properties of the essential oils of two *Guadua* Kunth species (Poaceae-Bambusoideae)** |
| **PP12** | *Eisuke Kuraya* (Japan) | **Chemical investigation of the volatile compounds of *Alpinia zerumbet* leaves using DH-TD-GC/MS** |
| **PP13** | *Marcia Ortiz M. Marques* (Brazil) | **Composition and antimicrobial activity of the essential oils from a wide range of species from the Atlantic Rainforest in Brazil** |

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| **PP14** | *Valtcho Zheljazkov* (USA) | **Carotenoid-related volatile compounds of tobacco (*N. tabacum* L.) essential oils** |
| **PP15** | *Isiaka Ogunwande* (Nigeria) | **Chemical constituents of essential oils from some Vietnamese plants** |
| **PP16** | *Noha Mahmoud Ayoub* (Turkey) | **Essential oil composition of *Salvia sclarea* L. aerial parts and its AChE inhibitory properties** |
| **PP17** | *José Eduardo Brasil P. Pinto* (Brazil) | **Influence of light quality on *in vitro* growth and essential-oil composition of *Chenopodium ambrosioides* L.** |
| **PP18** | *Marina Dimitrijević* (Serbia) | **Anticandidal activity of *Inula helenium* root essential oil: synergistic potential, anti-virulence efficacy, and mechanism of action** |
| **PP19** | *Eisuke Kuraya* (Japan) | **Improving the efficiency of essential-oil extraction from *Abies sachalinensis* with an underwater shockwave pretreatment** |
| **PP20** | *Barbara Horváth* (Hungary) | **Preparation and *in vitro* diffusion study of essential oil Pickering emulsions stabilized by silica nanoparticles for *Streptococcus mutans* biofilm inhibition** |
| **PP21*** | *Asit Ray* (India) | **Quality evaluation of *Hedychium coronarium* essential oils by GC-MS fingerprinting associated with chemometrics** |
| **PP22** | *Éva Zámboriné-Németh* (Hungary) | **Small changes in the distillation method result in variable quality of yarrow (*Achillea collina*) essential oil** |
| **PP23** | *Remigius Chizzola* (Austria) | **Volatiles from *Smyrnium perfoliatum* (Apiaceae) grown in Austria** |
| **PP24** | *Elif Güzel* (Turkey) | **Essential-oil composition of *Isatis floribunda* Boiss. ex Bornm. aerial parts from Turkey** |
| **PP25** | *Mercedes Pérez-Recalde* (Argentina) | **Lavandin essential oil combined with the biopolymer PHBV, poly(3-hydroxybutyrate-*co*-3-hydroxyvalerate), for wound treatment** |
| **PP26** | *Ivan Ilić* (Serbia) | **Oregano (*Origanum vulgare*) essential oil prevents L-arginine-induced rat ileum villi damage** |
| **PP27** | *Dušan Sokolović* (Serbia) | **Effects of a combined thymol and carvacrol application on rat kidney damage parameters after L-arginine application** |
| **PP28** | *Olivera Politeo* (Croatia) | **Medicinal plant *Mentha pulegium* L.–chemical profile and biological activity of its essential oil** |
| **PP29** | *Petras Rimantas Venskutonis* (Lithuania) | **Essential oils from five *Nepeta* spp. cultivated in Lithuania and toxicological evaluation of their main components** |
| **PP30** | *Branimir Pavlić* (Serbia) | **Hydrodistillation versus microwave-assisted hydrodistillation of sage herbal dust: kinetics, chemical profile and bioactivity** |

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| **PP31** | *Patrizia Rubiolo* (Italy) | **High efficiency microfabricated planar columns for analysis of real-world samples of essential oils and plant volatile fraction** |
| **PP32** | *Patrizia Rubiolo* (Italy) | **From medicinal and aromatic plants to herbal teas: quantitative determination of volatile bioactive secondary metabolites** |
| **PP33** | *Patrizia Rubiolo* (Italy) | **Adulterated essential oils: when the chemical composition compliance with the European Pharmacopoeia misleads** |
| **PP34** | *David Lee Nelson* (Brazil) | **Effect of the essential oil from *Cantinoa carpinifolia* (Benth.) Harley & J.F.B.Pastore on efflux of potassium ions from *Escherichia coli* and *Staphylococcus aureus* strains** |
| **PP35** | *David Lee Nelson* (Brazil) | **Chelating effect of carvacrol and the oregano essential oil** |
| **PP36** | *Cícero Deschamps* (Brazil) | **Cones and essential-oil production in hop with different nitrogen levels in the south of Brazil** |
| **PP37** | *Juergen Wanner* (Germany) | **Dermal application of oregano essential oil against recurrent urinary tract infections: an *in vivo* human pilot study** |
| **PP38** | *Jelena Arsenijević* (Serbia) | **Comparison of hydrodistillation (HD), microwave-assisted hydrodistillation (MHD) and supercritical fluid extraction (SFE) for the isolation of volatiles from chamomile flower** |
| **PP39** | *Daniel Jan Strub* (Poland) | **Microbial growth inhibition by oximes derived from natural volatile carbonyl compounds** |
| **PP40** | *Jelena Radović* (Serbia) | **The analyses of commercial tea tree oils** |
| **PP41** | *Jelena Radović* (Serbia) | **The composition of the essential oils of *Acorus calamus* L. rhizomes from different habitats** |
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## PP1. The influence of two Lamiaceae essential oils on dementia-related symptoms in animal models

*Tadaaki Satou*[1]*

*Keywords*: rosemary essential oil, thyme essential oil linalool chemotype, Y-maze test, elevated plus-maze test

Dementia is a major problem for aging societies. Several essential oils (EOs) used for aromatherapy have been claimed to be effective for dementia-related behavioral problems, but there is insufficient scientific evidence to fully back up these claims. In order to gain further insight into the influence of plant EOs on dementia symptoms, we report on the results of experiments in relevant animal models with two Lamiaceae essential oils of known composition (*Thymus vulgaris* L. linalool chemotype, and *Rosmarinus officinalis* L.). In experiment 1 [1], the permeability of the blood brain barrier (BBB) by EO constituents of *T. vulgaris* was investigated in the state of brain dysfunction and stress. In experiment 2 [2], *R. officinalis* EO was assessed for its effects on Alzheimer's type dementia symptoms. During the course of experiment 1, inflammation-induced mice (intraperitoneally administered with polyinosinic:polycytidylic acid (poly I:C)) were exposed to thyme EO vapors to evaluate the relationship between the BBB permeability of linalool and terpinene-4-ol and stress. Whereas in experiment 2, Alzheimer's type dementia model mice (intraperitoneally administered with scopolamine) that inhaled rosemary EO were tracked for improvements of their cognitive function in a Y-maze test. The results of experiment 1 showed that stress increased the passage of inhaled thyme EO components through the BBB. Experiment 2 provided evidence that the inhaled rosemary EO improved mice cognitive function. One can expect that the results concerning the effect of rosemary EO on the cognitive function of experimental animals will accelerate future research on EOs that affect dementia.

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# PP2. Cannabis terpene profiling in therapeutic products by means of gas chromatography coupled with mass spectrometry

*Margita Utczás*[1,2]*, Emanuela Trovato[2], Filippo Alibrando[2], Federica Vento[2], Luigi Mondello[2,3]

*Keywords*: cannabinoids, terpenes, GC-MS, linear retention index

It is well-known that cannabinoids provide non-toxic medical benefits and have an effective role in the treatment of chronic pain due to their interaction with the endocannabinoid system. Recently, in addition to the "classical" therapeutic usage, like inhalation or ingestion of cannabis, newer ways of cannabinoid-based products utilization are also being developed. The skin application of topicals including balms, lotions, and oils that are infused with active cannabinoids is a minimally invasive method for the medical cannabis use and allows them to be absorbed directly into the affected area for faster and more focused relief.

According to the terpene profile, the medicinal effect of cannabinoids can change significantly. Terpenes, in fact, have various roles: can make the adsorption of cannabinoids faster, or lessen their effect, interact with cannabinoids, decrease the side-effects of the cannabinoid therapy, and help to relax and calm the patient.

Gas chromatography-mass spectrometric (GC-MS) analysis is a powerful analytical tool for detailed characterization of the volatile fractions of any kind of complex sample. For the identification, mass spectral databases are used, but in many cases, misidentification could occur due to the high spectral similarity of terpenes. The Linear Retention Index (LRI) approach combined with conventional mass spectral search provide a more reliable solution for peak assignment. The FFNSC 4.0 (Flavour and Fragrance Natural and Synthetic Compounds), a dedicated MS Library with embedded LRI information, including almost all of the 140 known cannabis terpenes can be a great support in terpene profiling, thereby also in the optimization of the therapy.

Aroma constituents of cannabinoid-containing medicinal products were analyzed by GC-MS. To obtain the characteristic volatile fraction, sample preparation method was optimized for each sample type. Terpenes were identified using FFNSC 4.0 database.

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## PP3. The use of essential oils for antimicrobial food packaging

*Filomena Silva*[1,2]*, Celia Domeño[2], Cristina Nerín[3]

*Keywords*: essential oils, antimicrobial activity, active food packaging

Despite extensive efforts to control microbial and chemical contamination of foods, foodborne infections continue to have a significant economic and social impact. Given that 99.8% of all food and beverages will have to be encased in some sort of packaging during their existence, food industry is constantly evolving by introducing new technologies that enhance product quality and shelf-life. In this work we will focus on the development of antimicrobial food packaging as a means to control microbial contamination of foods and the transmission of foodborne pathogens to humans while also improving product shelf-life. Specifically, we propose to incorporate essential oils and their major compounds in several packaging materials ranging from paper to plastics. Cinnamon essential oil-based paper packages proved to be effective in controlling mold growth on cherry tomatoes [1]; while plastic-based ones displayed *in vitro* efficacy against several bacteria and fungi (*Escherichia coli* O157:H7, *Saccharomyces cerevisiae*, *Aspergillus flavus*, *Penicillium roqueforti*, *Penicillium expansum*, among others) and were able to successfully increase the shelf-life of tomato puree, bakery products, fruit jams and sliced bread [2]. Oregano essential oil-based antimicrobial food packages proved to be effective in reducing *E. coli* O157:H7 counts both *in vitro* and in sheep cheese [3]. Antimicrobial labels containing benzyl isothiocyanate proved to be effective in reducing *Aspergillus ochraceus* growth as well as the production of ochratoxins A and B [4]. Overall, these packaging systems were able to increase shelf-life and reduce microbial contamination in a vast array of food products, suggesting their commercialization as active food packages.

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## PP4. Chemical analyses of truffle flavored (*Tuber* spp.) olive oils on the Greek market with HS-SPME

*Eleni Stavraki*[1]*, Konstantia Graikou [1], Ioanna Chinou[1]

*Keywords*: *Tuber magnatum*, *T. melanosporum*, truffle aroma, olive oils

Truffles are subterranean edible fungi of the genus *Tuber* (Ascomycota, Pezizales), with a high commercial interest and economic value due to their unique aroma [1]. There are a number of foods flavored with truffles, such as oils etc. The aroma profile of such flavored foods has been studied thoroughly during the last decades. In the framework of this study, 5 truffle olive oils from the Greek market were investigated, coming from white (*T. magnatum*) and black (*T. melanosporum*) truffles. All samples were analyzed by Headspace Solid-Phase Micro-Extraction (HS-SPME) coupled with Gas Chromatography-Mass Spectrometry (GC-MS) and a total of 31 metabolites were identified, including a variety of sulfur-containing volatiles. 2,4-Dithiapentane, well known as a volatile chemical marker of white truffles [2], was detected in high concentrations in both white and black truffle olive oils, however, probably as the main constituent of synthetic flavor additives. Furthermore, other artificial sulfur-containing compounds were identified in the oils available in the market, e.g. 1-propanethiol, diallyl sulfide, and allyl isothiocyanate, which have not been detected previously in other truffle olive oils but have been reported among the volatiles of *Allium* spp. [3,4] and *Brassica nigra* [5], respectively. In conclusion, this study confirmed that all studied truffle olive oils from the Greek market are produced by the addition of synthetic aroma compounds. These flavors are of low cost, highly effective olfactorily [6], and of low toxicity, used widely according to European regulations in order to imitate the aroma of truffles.

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## PP5. On the subcritical extraction of *Rosa damascena* Mill.

*Ana Dobreva*[1]*, Ivayla Dincheva[2], Nenko Nenov[3]

*Keywords*: *Rosa damascena* Mill., subcritical extraction, yield, composition

Subcritical extraction of *Rosa damascena* Mill. has been performed with Freon R143a [1]. The pressure and duration of the process have been studied to obtain the highest possible yield. It was found that a short-time triple extraction at low pressures of 5-6 bar resulted in the highest yield–0.151%. The chemical composition of the product revealed a high terpene/scent content: β-phenylethyl alcohol (25.6-54.1%), citronellol (1.9-2.3%), geraniol (1.2-3.8%) and nerol (1.8-2.9%). The distribution of paraffins' content was: nonadecane (2.7-4.9%), nonadecene (3.0-5.6%), eicosane (4.4-9.4%) and heneicosane (4.4-9.8%). The deviations in the constituents of the day product and the year batch production have been discussed. The yield and composition are compared with other rose aromatic products [2,3].

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## PP6. The impact of soil herbicides on the yield and quality of lavender (*Lavandula angustifolia* Mill.) essential oil

Desislava Angelova[1], *Ana Dobreva*[1]*, Ganka Baeva[1]

*Keywords: Lavandula angustifolia* Mill., varieties, herbicides, essential-oil composition

During the period 2014-2015, the herbicidal effect and the selectivity of isoxaflutole (Merlin 750 WG), oxadiargyl (Raft 400 SK), imazamox (Pulsar 40) and flumioxazine (Pledge 50 WP) were studied on lavender fields, Hemus and Jubilee varieties [1]. The present work focuses on the influence of low doses of the applied preparations on the yield and composition of the essential oil compared to the untreated control [2]. The results of a two-year study show that the treated lavender had a higher yield on average of 0.7-1.6 kg/decare (daa). The odoriferous ingredients were found to be: linalyl acetate (20.0-38.6%), linalool (20.6-46.2%), lavandulyl acetate (1.9-5.9%), 1,8-cineole (0.4-4.9%), and camphor (0.2-0.6%). The application of oxadiargyl resulted in greater changes in the composition of the Jubilee variety, whereas the Hemus variety was most influenced by isoxaflutole [3].

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# PP7. Volatiles characterization of different commercial honey types from the Azores (Portugal)

*Alexandra M. Machado*[1]*, M. Graça Miguel[2], Miguel Vilas-Boas[3], A. Cristina Figueiredo[1]

*Keywords*: honey, Azores, volatiles, *Pittosporum*

Honey and beekeeping products are usually consumed due to their nutritional and therapeutic properties, being also used in fragrances or cosmetics [1]. The Azores have a specific endemic flora as well as climate and soil conditions that allow the production of a unique honey classified as Protected Designation of Origin (PDO), with multifloral or *Pittosporum undulatum* Vent. ("incenso") botanical origin [2]. As part of a research program aiming to evaluate the existence of specific honey volatile markers, this work reports the volatile profile of eight commercial honeys from the Azores (São Miguel, Santa Maria, Terceira and Pico). The volatiles were isolated by hydrodistillation for 1 h and analysed by gas chromatography and gas chromatography-mass spectrometry. The acyclic hydrocarbons *n*-nonadecane, *n*-heneicosane, *n*-tricosane, *n*-pentacosane, *n*-heptacosane and *n*-nonacosane dominated in all samples. Saturated fatty acids were also identified, namely decanoic and hexadecanoic acids. 2-Furfural, benzaldehyde, phenylacetaldehyde, phenylethyl alcohol, limonene and oxygen-containing terpenes, *cis*- and *trans*-linalool oxides, linalool, α-terpineol and α-, β- and γ-eudesmol, were detected in lower amounts. Although no previous studies described the volatiles of *Pittosporum* flowers from the Azores, a comparison with the volatiles isolated from the mainland *Pittosporum* flowers [3] showed that limonene, linalool, α-terpineol and α-eudesmol were present both in the Azorean honey samples (0.05-0.5%) and in the mainland flowers (0.05-2.2%). Further studies will aim at evaluating both the volatiles of honey from the main botanical origin, and well as the honey's biological properties.

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## PP8. New neryl esters from *Helichrysum italicum* essential oil

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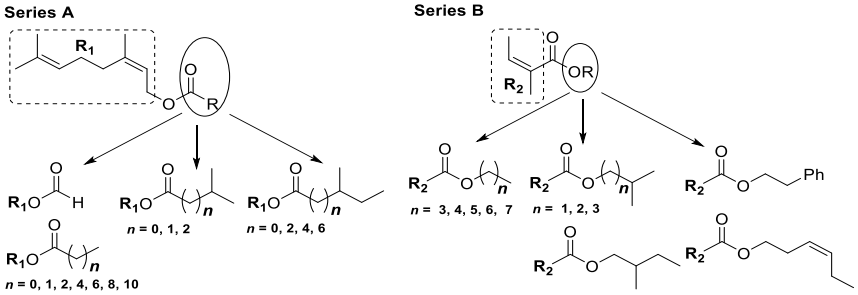
*Keywords*: *Helichrysum italicum*, essential oil, neryl esters, *anteiso*-medium chain fatty acid esters

*Helichrysum italicum* (Roth) G. Don (*Asteraceae*), commonly known as the everlasting or curry plant, is endemic to the Mediterranean region where at least 3 subspecies can be found. The typical subspecies (*italicum*) produces an essential oil rich in the acetate (≥ 30%) and propionate (≥ 5%) of nerol, and the characteristic β-diketones (≥ 10%). It is appreciated by perfumers because of the spicy saffron character well complemented with curry, nutty and celery facets [1]. As esters are an important group of aroma-active volatiles, in this work we aimed to study the composition of the ester fraction of the mentioned everlasting essential-oil chemotype. After chromatographic separations, our attention was focused on the ester fraction that contained numerous minor neryl and angeloyl esters undetectable in the direct GC-MS analyses of the unfractioned oil (series A and B, respectively; Fig. 1). Three esters of nerol and medium-chain *anteiso*-fatty acids ($C_7$, $C_9$ and $C_{11}$) represented new natural products, while several other esters (e.g. neryl decanoate and dodecanote, and phenethyl, heptyl and octyl angelates) have a rather restricted occurrence in the Plant Kingdom. Our study disclosed an extensive diversity of volatile esters present in the studied chemotype, some of which may contribute to the overall aroma-profile of the essential oil.

Fig. 1. Structures of neryl and angeloyl esters identified in *H. italicum* essential oil

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## PP9. Antimicrobial and anti-inflammatory potential of different immortelle essential-oil chemotypes

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*Keywords*: *Helichrysum italicum*, essential-oil chemotypes, antimicrobial activity, macrophage viability, principal component analysis (PCA)

*Helichrysum italicum* or immortelle (Asteraceae) essential oil has been widely used in alternative medicine for wound healing and other skin conditions such as hematoma and scars. It is possible that the therapeutic efficacy of this oil changes with the natural variability of the composition, i.e. existence of chemotypes, and due to various environmental factors (soil type, altitude, sun exposure, etc.) [1]. Herein we aimed to assess the relationship of the composition and the overall antimicrobial and anti-inflammatory potentials for 4 commercial immortelle oils containing differing amounts of neryl esters (23 : 43 : 12 : 21; oils 1, 2, 3, and 4, respectively), α-pinene (17 : 2 : 20 : 5), γ- and *ar*-curcumenes (19 : 14 : 16 : 15), and β-diketones (3 : 12 : 5 : 7). Oils 3 and 4 displayed higher antimicrobial activity compared to oils 1 and 2, showing a prominent anti-*Staphylococcus aureus* effect (MIC = 0.62 and 0.31 mg/mL, respectively). The tested strains were least susceptible (MIC ≥ 5 mg/mL) to the action of oil 1, rich in mono- and sesquiterpenic hydrocarbons. However, this oil, along with oil 3, showed the highest cytotoxicity toward macrophages ($LC_{50}$ ~ 0.14 mg/mL). Among the oil chromatographic fractions, those enriched in α-pinene and curcumenes displayed the highest cytotoxicity, but were inferior to the toxicity of the oils. The statistical (PCA) treatment of the obtained composition-activity data implied that the observed differences in activities among the tested oils were not only due to the different amounts of the major constituents, but also due to the presence of minor constituents (e.g. 2-methylbutyl angelate in the case of the anti-staphylococcal activity of the oils). Interestingly, based on literature data, the constituents that displayed strong negative correlations in the PCA matrix possess a lower antimicrobial potential than the tested oils. We found that immortelle oil efficiency as antimicrobial and anti-inflammatory agents strongly depends on its composition and is an outcome of synergistic action between its constituents.

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# PP10. Effect of macro- and micro-element-deficiency on growth and essential-oil composition of *Mentha arvensis L.* cultivated in solution

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*Keywords*: medicinal plant, hydroponic system, nutrient omission, fertilization

Because of its olfactory properties, the essential oil (EO) of *Mentha arvensis* L. is readily used in perfumery and cosmetics and has a great commercial value. However, the agronomic aspects of *M. arvensis* cultivation were not sufficiently studied. Herein, we assessed the effect of the absence of selected macro- and micronutrients on the growth and essential-oil composition of *M. arvensis* cultivated in solution. The experiment was completely randomized, with three replications and 12 treatments. Acclimated scions of *M. arvensis* were transferred into pots containing either the complete Hoagland & Arnon (HA) nutrient solution or modified HA solution, deficient in one of the following macro- or microelements: N, P, K, Ca, Mg, S, B, Cu, Fe, Mn and Zn. The experimental plot consisted of one plant per pot. Plants were cultured in the greenhouse under natural light for 45 days, during which air was supplied to the nutrient system and the nutrient solution was changed each week [1]. Plants were harvested at the end of the culture period and growth parameters (development and appearance of leaves, shoots, roots and the total dry weight) and leaf EO composition were evaluated. The results showed that the composition of the nutrient solution exerted a significant effect on all of the growth parameters and essential-oil chemical profile. With regard to the total dry matter, the order of limiting nutrients was N=Ca>P=B>K=S>Fe=Mg>Zn=Mn>Cu=HA. The most pronounced changes in the *M. arvensis* development were observed in the absence of N, P, Ca and B. The omission of Mn and Cu in the culture solution did not adversely affect the growth of *M. arvensis*. Omission of B, P, Ca, Mg and S from the nutritive solution resulted in a higher production of menthol, relative to the control.

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# PP11. Chemical composition and antimicrobial properties of the essential oils of two *Guadua* Kunth species (Poaceae-Bambusoideae)

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*Keywords*: Bamboo, essential oil, antimicrobial activity, *Guadua angustifolia*, *G. chacoensis*

Bamboos are described as one of the most important renewables, easily obtained, and valuable of all forest resources. Brazil is the country with the greatest diversity of bamboo species in the New World [1]. One of the most important bamboo groups growing in South America belongs to the *Guadua* genus, from which two species, *G. angustifolia* Kunth. and *G. chacoensis* (Rojas Acosta) Londoño & P.M. Peterson, are morphologically closely related. Due to the taxonomic difficulties presented by the *Guadua* complex, the main objective of this work was to evaluate the potential of their volatile oils for distinguishing the closely related species and to evaluate new potential applications for these plants. Leaves of the taxa were collected at an Experimental Unit from the Agronomical Institute from Campinas (IAC) located in Tatuí-SP. The essential oils were obtained by hydrodistillation for 4 h, and component identification was performed by GC/MS [2]. The yields were found to be 0.027% and 0.00079% (w/w), for *G. angustifolia* and *G. chacoensis*, respectively. Terpenes and terpene-related compounds accounted for most of the compositions of the two samples. The major compounds of *G. angustifolia* oil were hexahydrofarnesyl acetone (23.1%) and (*Z*)-phytol (21.3%), while *G. chacoensis* oil was characterized by (*E*)-β-ionone (8.8%), hexadecanoic acid (6.8%), hexadecenoic acid (6.5%), (*Z*)-phytol (5.3%) and (*E*)-α-ionone (5.0%). The antimicrobial activity was assayed by a microdilution method in microplates [2] against *Aspergillus brasiliensis*, *Candida albicans*, *Escherichia coli*, *Pseudomonas aeruginosa* and *Staphylococcus aureus*; none of the oils exerted any considerable activity (MIC > 250 µg/mL), as only extracts with MIC < 100 µg/mL can be considered as candidates for developing new antimicrobial agents [3].

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# PP12. Chemical investigation of the volatile compounds of *Alpinia zerumbet* leaves using DH-TD-GC/MS

*Eisuke Kuraya*[1]*, Akiko Touyama[1], Kenta Watanabe[1]

*Keywords*: *Alpinia zerumbet*, dynamic headspace-thermal desorption-GC/MS

The aromatic perennial plant *Alpinia zerumbet* (Pers.) Burtt & Smith (Zingiberaceae) grows in Japan, from the southern Kyushu to the Ryukyu Islands. Recently, interspecific hybridization of *Alpinia* spp. was reported in Taiwan. We have demonstrated that the floral volatiles of *A. zerumbet* differ between individual plants [1]. We also showed that the yield, content of the major volatile compounds, enantiomeric ratio of some monoterpenes, and antioxidant activities of the *A. zerumbet* leaf essential oils varied significantly among individual plants [2], which reflected genetic variability within the species. However, this trend needed to be demonstrated with more individuals. Unfortunately, a large quantity of leaves is necessary to obtain sufficient essential oil to investigate the differences in the chemical composition of the oils among individuals, because *A. zerumbet* leaves yield only a small amount of the essential oil upon hydrodistillation (0.01–0.07%). Prompted by this, here, we combined the dynamic headspace method with thermal desorption-gas chromatography-mass spectrometry (DH-TD-GC/MS). For this method, a small piece of a leaf is used and sampling is possible directly in the field. The aims of this study were to test the effectiveness of this DH-TD-GC/MS method and reveal the variation in the chemical composition of the essential oils of the leaves among the individual plants.

*Alpinia zerumbet* leaves were collected from Okinawa and Ie (16 and 22 samples, respectively), the Ryukyu Islands, between May and October 2017. The leaves were oven-dried (40–45 °C) to a moisture content of 10% or less, and 0.5 g of the dried leaves and stems from individual plants were septum-sealed in a 27-mL gas-tight vial. After introducing air through the activated carbon trap into the vial, volatiles were aspirated by a minipump and adsorbed to Tenax TA (60/80 mesh, 130 mg) for 10 min at 60 °C. Chemical analysis was performed using a TD-GC/MS system. The major volatiles identified in this study (α-pinene, camphene, limonene, β-phellandrene, 1,8-cineole, *p*-cymene, camphor, linalool, and cryptone) well represented the characteristics of the essential oil of the leaf. The aroma profile obtained here also confirmed that the volatiles in the leaves clearly differed among individual plants. These observations suggest the plausibility of selecting lineages of *A. zerumbet* to optimize the future production of valuable essential oils.

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## PP13. Composition and antimicrobial activity of the essential oils from a wide range of species from the Atlantic Rainforest in Brazil

*Marcia Ortiz M. Marques*[1]*, Crislene V. Perigo[1], Lenita L. Haber[2], Maria A. R. Vieira[1], Roselaine Facanali[1], Roseli B. Torres[1], Luís C. Bernacci[1], Vera Quecini[3]

*Keywords*: antimicrobial activity, essential oil, monoterpene, rainforest, sesquiterpene

The Neotropical Atlantic Forest is considered one of the world´s richest biome in plant and animal diversity, with high frequency of endemic species. In this work we studied the chemical composition of the essential oils from 41 plants, belonging to 13 botanical families, from distinct locations of the Atlantic rainforest in the state of São Paulo, Brazil. The essential oils were isolated by hydrodistillation and their compositions were determined by GC-MS. Additionally, the antibacterial activity of the oils was investigated by growth-inhibition agar-diffusion assays, in the case of four bacterial species (*Staphylococcus aureus, S. epidermidis, Corynebacterium xerosis* and *Escherichia coli)*, while minimum inhibitory concentrations (MIC) were determined for both bacteria and fungi. For the inhibition halo analyses, *Melaleuca* sp. essential oil and cefotaxime were used as positive controls, whereas sterile mineral oil was used as the negative control. The analyses showed that the most abundant compounds were mono- and sesquiterpenes, although *Lauraceae* and *Myrtaceae* species oils also contained phenylpropanoids and methyl ketones, respectively. Hierarchical clustering analyses demonstrated that the mono- and sesquiterpene composition of the investigated oils was not significantly determined by the botanical family, forest location or seasonality alone; alternatively, the combination of these factors determines the chemical phenotype. The vast majority of the isolated essential oils exhibited an *in vitro* activity against Gram-negative and Gram-positive bacterial species and the composition of the bacterial cell wall is the principal factor affecting the extent of the biological activity of the investigated essential oils. The contents of the detected monoterpenes positively correlated with the observed biological activity against the given bacterial strains. Elevated contents of α- and β-pinene positively correlated with the increased inhibition of *Staphylococci* growth, whereas increased levels of germacrene D were associated with the antibacterial activity against *C. xerosis*.

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# PP14. Carotenoid-related volatile compounds of tobacco (*N. tabacum* L.) essential oils

Venelina Popova[1], Tanya Ivanova[1], Tsvetko Prokopov[1], Milena Nikolova[1], Albena Stoyanova[1], *Valtcho D. Zheljazkov*[2]*

*Keywords*: tobacco, essential oils, volatile compounds, carotenoids

Tobacco (*Nicotiana tabacum* L.) aroma is an important quality attribute of tobacco and consists of a variety of minor components, among which carotenoid degradation products. The transformation of tobacco carotenoids (mainly lutein and β-carotene) occurs both in fresh green leaves and during curing, thus producing nearly 100 different short-chained metabolites. The three major tobacco types traditionally produced in Bulgaria and used as blends in the manufacture of cigarettes, include oriental (*OR*), flue-cured Virginia (*FCV*), and Burley (*BU*). High-quality Bulgarian oriental tobacco is also processed to obtain concrete and absolute, which are used in fine perfumery. Therefore, the objective of this work was to determine the content of the most important fragrance-shaping carotenoid degradation products in the essential oils (EOs) of the three types of Bulgarian tobacco, and to compare them with other aroma products from tobacco.

The content of total carotenoids and β-carotene was highest in the air-cured *BU* tobacco (22.23 and 20.34 mg/100 g, respectively), followed by the sun-cured *OR* (13.60 and 12.09 mg/100 g in variety "Plovdiv 7" (*Pd7*); 6.27 and 5.45 mg/100 g in "Krumovgrad" (*Kr*), and *FCV* (5.93 and 3.73 mg/100 g). Tobacco EOs were obtained by hydrodistillation in an acidified medium, and the yields were: *FCV* - 0.23%; *BU* - 0.26%, *OR* - 0.44% *(Kr)* and 0.30% *(Pd 7).* All EOs were light yellow and had a sharp odor: *FCV* – very intense, balsamic, woody with earthy undertones; *BU* – mild woody with balsamic and floral-like undertones, and *OR* – very green with slightly smoky and mossy-like and honey-like undertones. The main aroma-impact compounds from carotenoid degradation identified in the EOs (by GC-MS) were as follows: *FCV* - α-ionone (1.4%), dihydro-β-ionone (2.2%); β-damascenone (2.9%); *BU* - α-ionone (1.9%), dihydro-β-ionone (3.1%); β-damascenone (3.5%); *OR(Kr)* - α-ionone (0.9%), β-ionone (2.8%), dihydro-β-ionone (5.9%); β-damascenone (1.6%); *OR (Pd7)* - α-ionone (4.3%), dihydro-β-ionone (5.2%); β-damascenone (3.7%). Compared to published data for other tobacco EOs, these results reveal some differences in damascone derivatives, explainable by plant material origin and processing conditions. Ionone and its derivatives were not identified in the aroma extraction products concrete and resinoid from the same tobaccos, neither in the absolute from the Bulgarian tobaccos. The results agree with previous findings about the effect of thermal degradation, pH of the medium and other factors on carotenoid transformations in plant materials. The study provides an insight into the composition of EOs from the tobaccos produced in Bulgaria, and may be of interest to the fragrance industry.

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# PP15. Chemical constituents of essential oils from some Vietnamese plants

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*Keywords*: *Alphonsea tonquinensis*, *Schefflera myriocarpa*, *Siliquamomum tonkinense*, *Anoectochilus setaceus*, *Codonopsis javanica*, *Aristolochia kwangsiensis*, essential oils, terpenes

Vietnam, like any other tropical country of the world, is blessed with many medicinal plants and herbs. However, a literature search has revealed that the chemical compositions of the majority of these plants, as well as their biological potentials, have not been documented. The present paper aimed to report the chemical constituents identified in the essential oils of some plants grown in Vietnam. The essential oils were obtained by hydrodistillation in accordance with the Vietnamese Pharmacopoeia. The chemical constituents of the oils were analyzed by gas chromatography and gas chromatography-mass spectrometry on an HP-5MS column. The main compounds in the leaf oil of *Alphonsea tonquinensis* A.DC. (Annonaceae) were β-caryophyllene (27.8%), β-elemene (15.6%) and caryophyllene oxide (14.5%). The stem oil was comprised mainly of germacrene D (17.4%), β-caryophyllene (9.9%), α-pinene (9.5%), β-elemene (9.3%) and β-pinene (9.2%). The principal compounds identified in the leaf, bark and stem oils of *Schefflera myriocarpa* Harms (Araliaceae) were mainly monoterpenes represented by α-pinene (17.1-21.2%), α-phellandrene (9.2-27.4%) and limonene (19.8-36.8%). In addition, methyl eugenol (10.4%) was found in the bark. *Siliquamomum tonkinense* Baill. (Zingiberaceae) yielded a leaf oil whose major compounds were β-pinene (29.3%), α-pinene (15.7%), and sabinene (14.6%), while 1,8-cineole (19.1%), γ-terpinene (14.9%), *o*-cymene (14.0%), and α-pinene (12.5%) were the main compounds present in the rhizome oil. The major components of the leaf oil of *Anoectochilus setaceus* Blume (Orchidaceae) were α-cadinol (17.1%), (*E*,*E*)-farnesol (14.0%) and terpinen-4-ol (11.0%) while β-pinene (20.8%) and α-pinene (15.4%) were the main compounds identified in the oil of *Codonopsis javanica* (Blume) Hook.f. & Thomson (Campanulaceae). However, the dominant compounds of the oil of *Aristolochia kwangsiensis* Chun & F.C.How ex S.Yun Liang (Aristolochiaceae) were sabinene (34.8%), β-caryophyllene (8.8%) and terpinen-4-ol (8.6%). To the best of our knowledge, this is the first report on the essential-oil compositions of these species. The chemotaxonomic importance of the results would also be discussed.

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# PP16. Essential oil composition of *Salvia sclarea* L. aerial parts and its AChE inhibitory properties

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*Keywords*: essential oil, *Salvia sclarea*, AChE, spathulenol, linalyl acetate

Previously, the hydrodistilled essential oils of the aerial parts of wild-growing *S. sclarea*, originating from two localities in Greece, were analyzed by GC-MS and it was found that the oils were rich in linalyl acetate, linalool and geranyl acetate [1]. The current study aims to provide information on the essential-oil composition of the aerial parts of *S. sclarea* from Turkey. The essential oil was obtained by hydrodistillation from air-dried aerial parts of the plant, collected in Turkey, using a Clevenger-type apparatus in the duration of 3 h. The essential oil yield was 0.23 mL per 100 g of plant material. The essential oil was diluted with *n*-hexane 1:10 (*v*/*v*) and used as such for GC-MS analysis. The essential oil was analyzed with an Agilent 5977 MSD GC-MS system operating in EI mode; injector and MS transfer line temperatures were set at 250 °C. Splitless injection was used in the analysis. Innowax FSC column (60 m x 0.25 mm, 0.25 µm film thickness) and helium as the carrier gas (1 mL/min) were used in GC-MS analyses. The oven temperature program was: 60 °C for 10 min and then raised to 220 °C at a rate of 4 °C/min, afterward the temperature was kept constant at 220 °C for 10 min and then raised to 240 °C at a rate of 1 °C/min. Mass spectra were recorded at 70 eV with the mass range *m/z* 35-425. Relative amounts of the separated compounds were calculated from the integration of the peaks in MS chromatograms. Identification of essential-oil components was carried out by comparison of their retention indices (RI), relative to a series of *n*-alkanes ($C_5$ to $C_{30}$), with the literature values, as well as by mass spectral comparison. The aerial parts essential oil of *S. sclarea* was found to contain linalyl acetate (9.8%), linalool (7.4%), germacrene D (6.0%), caryophyllene oxide (6.0%), β-caryophyllene (5.6%), α-terpineol (4.3%), and spathulenol (3.4%). The obtained results were in general accordance with the results given in the literature. Additionally, AChE-inhibitory property of the essential oil was investigated and the oil was found to inhibit AChE activity by 11.23 ± 0.003% ($n$ = 3) at a concentration of 1 mg/mL.

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# PP17. Influence of light quality on *in vitro* growth and essential-oil composition of *Chenopodium ambrosioides* L.

*José Eduardo Brasil P. Pinto*[1*], Alexandre Alves de Carvalho[1], Suzan Kelly Vilela Bertolucci[1]

*Keywords*: medicinal plant, blue light, red light, micropropagation

*Chenopodium ambrosioides* L. (*CA*) is a medicinal plant extensively used for its anthelmintic, anti-inflammatory, antileishmanial and antidiarrheal properties. One of the most important factors that regulates the growth and development of plants *in vitro* is light. Therefore, the aim of this study was to determine how spectral composition of light influences *in vitro* growth and chemical composition of *CA* essential oil (EO). To do that, nodal segments of *CA* were inoculated in a growth medium and cultured for 40 days in a growth room with different diodes emitting lights: blue (B), red (R), white (W), combinations of blue and red (B:R=1:1; 2:1; 1:2, respectively) and cool white fluorescent lamp (F). The chemical profiles of *CA* plant specimens grown under lights of different quality were mutually compared using principal component analysis (PCA). The results of PCA showed significant light-quality-related variations in EO profiles (Fig. 1): monochromatic B light inhibited the biosynthesis of ascaridole, while W, B:R=1:2 and 2:1 lights promoted ascaridole production. The herein obtained results suggest that explants kept in a growth room with W or B:R=2:1 lights had optimal chemical profiles.

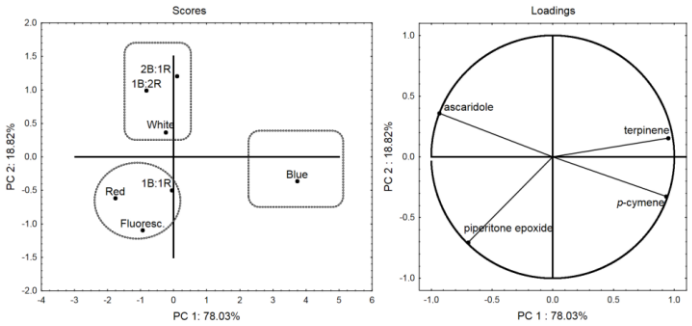


Fig. 1. PCA comparison of the chemical profiles of EOs obtained from *CA* grown under lights of different spectral composition

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## PP18. Anticandidal activity of *Inula helenium* root essential oil: synergistic potential, anti-virulence efficacy, and mechanism of action

Zorica Stojanović-Radić[1]*, *Marina Dimitrijević*[1], Milica Pejčić[1], Nikola Stanković[1], Marija Genčić[2], Milena Živković[2], Niko Radulović[2]

*Keywords*: *Inula helenium*, anticandidal, synergism, virulence factors

*Inula helenium* L. (elecampane) is a widely occurring perennial plant species in Europe and East Asia, belonging to the Compositae family. Roots of *I. helenium* have been traditionally used for the treatment of various diseases and it is officially listed in pharmacopeias as a diuretic, diaphoretic, expectorant and anthelmintic [1]. The present study investigated the anticandidal potential of *I. helenium* essential oil, isolated from roots and chemically characterized by GC and GC/MS. Antifungal efficacy was studied using the microdilution method and the determined minimal inhibitory concentrations (MICs) were further used to study a potential synergistic interaction of the oil and an antifungal. Together with this, the mode of action (sorbitol and cholesterol assays) and anti-virulence effects (antibiofilm, germ-tube reducing and phospholipase-inhibitory activities) were also investigated.

The results showed that the isolated essential oil contained alantolactone and isoalantolactone as the dominant constituents (65.8 and 25.5%, respectively). The obtained MICs varied among the strains, but the oil generally exhibited a high anticandidal potential (0.009-0.312 mg/mL). The oil displayed a high synergistic effect in combination with the antifungal agent nystatin. Experiments on the mode of action demonstrated that the oil affected the cell membrane function, due to the enhancement of the oil's activity (lowering of active concentrations) in the presence of sorbitol and cholesterol. Considering the virulence factors, the oil exhibited an antibiofilm activity, as well as a very high germ-tube reducing potential (93.3-100% at MIC). Additionally, a complete inhibition of the enzyme phospholipase in the presence of *I. helenium* root essential oil was demonstrated.

Based on the presented results, the essential oil of *I. helenium* can be considered as a good candidate for a natural agent that can be further explored in the sense of candidiasis treatment.

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## PP19. Improving the efficiency of essential-oil extraction from *Abies sachalinensis* with an underwater shockwave pretreatment

*Eisuke Kuraya*[1]*, Akiko Touyama[1], Osamu Higa[1], Yoshie Tsujikawa[2], Shigeru Tanaka[2], Shigeru Itoh[1]

*Keywords*: *Abies sachalinensis*, underwater shockwave pretreatment

*Abies sachalinensis* (Sakhalin fir) is a conifer species belonging to the family Pinaceae that is native to and widely distributed throughout Sakhalin Island, the southern Kurils (Russia), and northern Hokkaido (Japan). The essential oil of *A. sachalinensis* has been found to be an active removal agent, similar to γ-terpinene, myrcene, and β-phellandrene, which effectively remove nitrogen dioxide. Essential oils provide a relaxing effect; the use of essential oils is expected to improve overall air quality.
Underwater shockwaves generate instantaneous high pressure that reaches the entire cell and causes multiple cracks along the tracheids, causing the pit membrane to flake off through spalling destruction. These cracks function as permeation pathways [1]; this application was expected to result in a more effective essential oil extraction by subsequent steam distillation [2]. We, herein, introduce a novel application of this pretreatment process aimed at improving the efficiency of essential-oil extraction from *A. sachalinensis* leaves and branches. *A. sachalinensis* leaves and branches were oven-dried (40-45 °C) to a moisture content of 10% or less, and were subjected to the shockwave pretreatment or left untreated before essential-oil extraction by steam distillation. Chemical analysis was performed using gas chromatography-mass spectrometry. The essential-oil yields of raw untreated and untreated dried leaves were 5.1 and 2.4 g/kg of leaf dry weight (DW), respectively. Upon application of a 3.0 kV, 3.6 kJ shockwave, the essential-oil yield increased with the number of shockwave cycles; the yield was 32.7 g/kg DW after 10 cycles, a 13.6-fold increase compared to that of the untreated dried leaves. In addition, sesquiterpenes increased by more than 30-fold in content compared to that of untreated dried leaves. Thus, these results suggest that instantaneous high-pressure treatment, as a pretreatment for conventional steam distillation, has a distinct advantage in increasing the essential-oil yield and extracting the bioactive components. Furthermore, this method also can be used for the pretreatment of microwave essential-oil extraction or steam distillation under reduced pressure.

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# PP20. Preparation and *in vitro* diffusion study of essential oil Pickering emulsions stabilized by silica nanoparticles for *Streptococcus mutans* biofilm inhibition

*Barbara Horváth*[1], Viktória L. Balázs[2], Györgyi Horváth[2], Aleksandar Széchenyi[1]*

*Keywords*: essential oils, Pickering emulsion, emulsion preparation, *in vitro* diffusion study, biofilm inhibition

A long-standing problem in patient care is the ability of bacteria to form biofilms, including *Streptococcus mutans* biofilm on teeth or dental implants [1]. The essential oils have a proven ability for biofilm inhibition [2], but their direct use is limited due to their physical-chemical properties, such as the hydrophobicity and low water solubility. EOs are used as active ingredients in mouth care products, but the solvent components, e.g. DMSO or ethanol and surfactant as SDS or polysorbates in the case of emulsions, may influence the role and effect of EOs. To avoid the use of solvents and surfactants, we could use Pickering emulsions (PE), which are solid particle stabilized emulsions [3]. For this purpose, biologically inert solid particles are used, and this emulsion can be used for EO formulations. Besides emulsion stabilization, the solid particles may interact with biofilm [4] and targeted EO transportation can be also achieved. The aim of our work was to prepare silica nanoparticle stabilized PEs with thyme, clove, peppermint, and cinnamon EO, in order to enhance their bioavailability for potential biofilm inhibition. The droplet size and stability of PEs were determined by dynamic light scattering measurements. *In vitro* diffusion experiments have been performed on a model agar gel membrane with the PEs, conventional emulsions, and ethanolic EO solutions. EOs were used in the MIC/2 concentration against *S. mutans*. The results from diffusion experiments clearly show that EOs in PE form are more effective regarding the cumulative amount of EOs passed through the model membrane. Biofilm inhibition test has been also performed, where we have determined, that the EOs in PE form have a better biofilm inhibition effect then the solutions or conventional emulsions.

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# PP21. Quality evaluation of *Hedychium coronarium* essential oils by GC-MS fingerprinting associated with chemometrics

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*Keywords*: chemical fingerprint, chemometrics, GC-MS, *Hedychium coronarium*

*Hedychium coronarium* J. Koenig (Zingiberaceae) is a valued plant species due to its exquisitely fragrant essential oil. However, there is a significant diversity in essential oil yield and quality associated with the geographical origin of the plant. The aim of the present study is to establish a quality control chemical fingerprint and differentiate *Hedychium coronarium* essential oils of different geographical origin using chemometrics. A total of 50 samples collected from five different geographical regions (Odisha, West Bengal, Andhra Pradesh, Jharkhand and Assam) of India were analyzed by GC-MS. Forty four volatile constituents belonging to different classes were identified, among which *β*-pinene, eucalyptol, linalool and coronarin E were the predominant constituents. Thirteen shared chromatographic peaks were selected and the relative standard deviations of retention time and peak areas of these compounds were less than 0.2 and 3%, respectively. The correlation coefficients and overlapping peak ratio of each chromatogram to the simulative mean chromatogram was greater than 0.81 and 81.2%, respectively, thus indicating that the developed chemical fingerprint was very consistent. Chemometric techniques like hierarchical cluster analysis (HCA), principal component analysis (PCA) and stepwise linear discriminant analysis (SLDA) were applied to provide accurate classification and discrimination of *H. coronarium* essential oils of different origin. The HCA and PCA score plot clustered *H. coronarium* essential oils into 5 groups in accordance with their origin. By SLDA, 11 constituents with the best discriminating capacity were selected, and 4 discriminant functions (DFs) achieved a success rate of 100% in both classification and prediction, thereby revealing accurate discrimination of *H. coronarium* oils from different regions. These results suggest that GC-MS fingerprinting coupled with chemometrics could be an effective and reliable tool for identification and discrimination of *H. coronarium* of different geographical origin and for quality control.

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## PP22. Small changes in the distillation method result in variable quality of yarrow (*Achillea collina*) essential oil

*Éva Zámboriné Németh*[1]*, Klára Ruttner[1], Péter Radácsi[1]

*Keywords*: yarrow, extract, solvent, decantation, sesquiterpene

*Achillea collina* (Becker ex Rchb.f.) Heimerl (Asteraceae) is one of the yarrow species providing the chamazulene containing, characteristic blue essential oil by water distillation. The chamazulene content varies on a large scale [1,2]. Besides several other factors–like the determination of the species and taxon, geographical and ecological characteristics of the habitat, sampling, and GC analytical methods–which have been studied and discussed more frequently, the method of distillation and oil recovery might have a large influence on the quality of the oil, too. Unfortunately, the applied solvents, evaporation/drying methods and/or further dilution is almost never described accurately in manuscripts. Therefore, a well-established comparison and evaluation of the results is at least questionable. In our recent experiment, this aspect was investigated in detail. As plant material, a high chamazulene-containing strain of *A. collina* was used, selected and maintained at our experimental station. Dried flowering shoots were distilled in a Clevenger type apparatus: a) as in Pharmacopoeia Hungarica VII, b) as in Ph.Hg.VIII (=Ph.Eur.). For the second treatment, different solvents were applied for washing the sesquiterpene-rich oil of large viscosity: a) *n*-hexane, b) *n*-pentane, c) xylol, d) ethanol (96%), e) acetone. The recovered oil was analyzed a) immediately after the washing down, b) after the evaporation of the solvent–as for measuring the yield–diluted by different amounts of hexane again (resulting in 0.3, 1.0, 5.0, 10% concentrations) for the injection into the GC apparatus. The GC-MS analysis was carried out as in [3]. The results show that based on the above circumstances and factors, the number of GC peaks varied between 4 and 68. Chamazulene content of the oil samples changed between 45 and 78% of the total GC area percentage and a higher dilution rate of the extracts increased the ratio of chamazulene. Evaporation of the solvents resulted in a severe loss of volatile monoterpenes. At the same time, the proportion of α-bisabolol remained more constant (18-25%) but its ratio increased with the b-type of apparatus. Although internal standards might help quantification, however, the studied factors may influence severely the analytical results and any comparison. A well-established, standardized method of distillation and subsequent oil recovery process would be of high importance in the case of sesquiterpene-rich species.

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# PP23. Volatiles from *Smyrnium perfoliatum* (Apiaceae) grown in Austria

*Remigius Chizzola*[1]*

*Keywords*: essential oil, germacrene D, germacrone, furanosesquiterpenes, *Smyrnium perfoliatum*

*Smyrnium perfoliatum* L., perfoliate alexanders, is an umbelliferous biennial (Apiaceae) plant taxon native to the Mediterranean [1]. The rare occurrences of this species in Austria are possibly due to former uses as a cultural crop. For the present study, the plants were obtained from open areas of the Botanical Garden in Vienna and from a site near castle Liechtenstein, in the south of Vienna (Austria). *S. perfoliatum* is a plant low in essential oils. The oil contents decrease in the order: fruits, inflorescences, roots, stems, leaves. The essential oils were composed of sesquiterpenes, mainly germacrene D (6.5-32.7%) and germacrone (up to 28.6%) as well as of furanosesquiterpenes. Amongst these, 1β-acetoxyfuranoeudesm-4(15)-ene and 1β-acetoxyfuranoeudesm-3-ene were characteristic for the aerial plant parts. These compounds were also found in plants from Turkey [1] while the plants from the botanical garden Urbino (Italy) had aromadendrene and neryl isovalerate as the main oil compounds [2]. Plant roots from both Austrian sites contained curzerene = isofuranogermacrene and furanodienone as the main compounds in their volatile fractions. An SPME analysis of the headspace of fresh leaves and flowers revealed the presence of 80-84% of germacrene D and 2-4% of germacrene B while the furanosesquiterpenes were very low in relative amount.
In comparison, an inflorescence essential oil from *S. olusatrum*, alexanders, collected near Gubbio, Italy contained germacrone (23.4%), curzerene (18.4%) and myrcene (17.4%). A fruit oil from the same species originating from Lago Trasimeno, Italy, was composed of 1β-acetoxyfuranoeudesm-4(15)-ene (25.5%), α-pinene (18.2%), curzerene (8.4%), alexandrofuran (5.7%) and germacrone (5.0%). However, the evaluation of the volatile fractions bears an uncertainty as germacrone and some furanosesquiterpenes are reported to undergo partial thermal decomposition under the conditions of gas chromatography [3].

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# PP24. Essential-oil composition of *Isatis floribunda* Boiss. ex Bornm. aerial parts from Turkey

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*Keywords*: essential oil, *Isatis floribunda*, dodecanoic acid, nonacosane, hexadecanoic acid

There is just one article in the literature in regard to the essential-oil composition of *Isatis floribunda* Boiss. ex Bornm. (Brassicaceae). Previously, a flower and root extract of *I. floribunda* was reported to be rich in phenolic compounds, especially chlorogenic acid, *p*-coumaric acid and quercetin [1]. The current study aims to provide information about the essential-oil composition of aerial parts of *I. floribunda*. *Isatis floribunda* was collected from Ankara-Beypazarı. The essential oil was obtained by hydrodistillation of the air-dried aerial parts using a Clevenger apparatus for 3 h. The essential-oil yield was 0.03 mL per 100 g of plant material. The essential oil was trapped in *n*-hexane (1 mL) dried over anhydrous $Na_2SO_4$ and analyzed directly by GC-MS without further dilution. The essential oil was analyzed with an Agilent 5977 MSD GC-MS system operating in EI mode; injector and MS transfer line temperatures were set at 250 °C. Splitless injection was used in the analysis. Innowax FSC column (60 m x 0.25 mm, 0.25 µm film thickness) and helium as the carrier gas (1 mL/min) were used in GC-MS analyses. The oven temperature program was: 60 °C for 10 min and then raised to 220 °C at a rate of 4 °C/min, afterwards the temperature was kept constant at 220 °C for 10 min and then raised to 240 °C at a rate of 1 °C/min. Mass spectra were recorded at 70 eV with the mass range *m/z* 35-425. Relative amounts of the separated compounds were calculated from the integration of the peaks in MS chromatograms. Identification of essential-oil components was carried out by comparison of their retention indices (RI), relative to a series of *n*-alkanes ($C_5$ to $C_{30}$), with the literature values, as well as by mass spectral comparison. The aerial parts essential oil of *I. floribunda* yielded an essential oil that is rich in *n*-alkanes and saturated fatty acids. The major components of the essential oil were dodecanoic acid (28.6%), nonacosane (11.0%), hexadecanoic acid (10.0%), tetradecanoic acid (8.4%), methyl octadecanoate (4.8%), decanoic acid (4.6%), and hexahydrofarnesyl acetone (3.5%). We believe our study will stimulate further research on the chemistry of this species.

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## PP25. Lavandin essential oil combined with the biopolymer PHBV, poly(3-hydroxybutyrate-*co*-3-hydroxyvalerate), for wound treatment

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*Keywords*: lavender, PHBV, wound healing, keratinocytes, fibroblasts

In this work, poly(3-hydroxybutyrate-*co*-3-hydroxyvalerate), PHBV, was combined with lavandin essential oil (LavEO), from *Lavandula hybrida* grown in Argentina. Linalool (36%), linalyl acetate (29%) 1,8-cineole (6%) and camphor (6%) were its main compounds as analyzed by GC-MS. PHBV is a biodegradable copolyester from a bacterial source; PHBV porous scaffolds have been shown to be suitable for fibroblast and keratinocyte proliferation [1,2] and thus for skin regeneration. In addition, LavEO exhibits strong anti-inflammatory and antibacterial activity, what improves wound healing [4,5]. Purified monoterpenes and entire EOs have been combined with other biopolymers for different applications but scarcely for wound healing and never previously with PHBV [6]. PHBV porous membranes, 100-200 µm thickness, containing LavEO at 2, 4 or 8% m/m were obtained by an emulsion-solvent evaporation method. LavEO-PHBV membranes did not show cytotoxicity when tested on NIH/3T3 fibroblasts (according to the ISO 10993-5 standard). SEM membrane analysis showed, in all cases, a high level of porosity,~20% of the surface. Keratinocytes (KC) adhesion and proliferation were evaluated with the HaCaT cell line. Membranes containing 2 or 4% of LavEO, allowed KC proliferation of the same level as that of PHBV membrane controls. However, cells neither adhered to nor proliferated on membranes with 8% LavEO although their hydrophobicity, estimated by the contact angle, was similar to that of 4%-LavEO membranes. The reduction in the elastic modulus–determined by the dynamic mechanical analysis–due to the presence of LavEO, suggests its plasticizer effect (control E=305±10 MPa; 8%-LavEO membrane E=150±20 MPa). According to these results, 2 or 4% LavEO-PHBV membranes seem as a promising treatment, especially in the case of infected and chronic wounds, often arrested at the inflammatory phase.

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## PP26. Oregano (*Origanum vulgare*) essential oil prevents L-arginine-induced rat ileum villi damage

*Ivan R. Ilić*[1]*, Nikola M. Stojanović[1], Pavle Randjelović[1], Katarina Mitić[2], Dušan Sokolović[1], Milica Stevanović[2], Niko Radulović[2], Vesna Živković[1]

*Keywords*: *Origanum vulgare*, L-arginine, rat ileum mucosa

Oregano (*Origanum vulgare* L., Lamiaceae) is used for centuries as a culinary spice due to its food flavor enhancing properties and its specific aroma. Essential oil isolated from oregano is known to affect the function of the gastrointestinal system by causing stomach and throat smooth muscle relaxation. The present work aims to evaluate the potential protective effects of oregano essential oil in rat ileum intestinal mucosa injury, induced with high doses of L-arginine, by tracking pathological changes in ileum mucosa. Male Wistar rats, divided into four groups (n=6), were treated with 50 mg/kg of oregano essential oil or 200 mg/kg of allopurinol (xanthinoxidase inhibitor) 1 h before a single dose of L-arginine (3.5 g/kg). Two groups served as the controls – one treated with a single dose of L-arginine, while the second group of animals remained untreated. One day after the treatment, all animals were sacrificed and the segments of distal ileum were dissected and fixed in 10% buffered formalin solution. Afterward, the tissue was processed routinely in order to obtain paraffin molds which were further cut into 4-5 µm thin sections and stained with hematoxylin and eosin. Microscopic analysis of the control group ileum revealed short and cylindrical villi, with great resemblance to fingers, with no pathological substrate present. Ileum villi from the group of animals treated only with L-arginine appeared swollen, with the villi tip significantly dilated. Also, in the lamina propria, a large number of leucocytes were visible. The application of both allopurinol and oregano essential oil was able to prevent such significant alterations in the intestinal villi appearance (both in its intensity and frequency) and to reduce the number of leucocytes that migrated to the lamina propria. The detected activity can possibly be attributed to numerous oil constituents found in this essential oil, but predominantly to its major constituents thymol and carvacrol.

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## PP27. Effects of a combined thymol and carvacrol application on rat kidney damage parameters after L-arginine application

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*Keywords*: thymol, carvacrol, kidney damage, NGAL

Thymol and carvacrol are two frequently abundant volatile monoterpene phenols found as constituents of different, widely used medicinal plants mainly belonging to the Lamiaceae family. The two compounds were previously proven to possess a large number of pharmacological/toxicological activities, including the nephroprotective activity. The present study aims to evaluate the nephroprotective potential of the two mentioned monoterpenes in L-arginine-induced rat kidney damage model. The potentials of thymol and carvacrol to alleviate kidney impairment were investigated using a different serum (urea, creatinine, sodium, potassium) and homogenate (neutrophil gelatinase-associated lipocalin-NGAL) parameters that reflect kidney tissue damage. Significant rat kidney damage, increased serum urea, creatinine, sodium and potassium levels, as well as NGAL tissue activity, followed the application of L-arginine (3.5 g/kg). Thymol (10 mg/kg), carvacrol (10 mg/kg) or their combination (1:1, *w/w*, 10 mg/kg) application prior to L-arginine reduced the kidney tissue damage based on the determined values of the previously mentioned parameters. The activity of the combination of the two monoterpenes was found to be more pronounced than the activity of the individual ones at the same total dose. These differences were clearly visible in the urea and potassium serum levels and in the NGAL tissue activity obtained from the corresponding experimental groups. Such greater nephroprotective potential of the combination of the two compounds could be attributed to a possible synergistic effect of the two volatile phenols, since they were proven alone to both possess antioxidant, anti-inflammatory, immunomodulatory, anti-apoptotic, etc. activities.

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# PP28. Medicinal plant *Mentha pulegium* L.–chemical profile and biological activity of its essential oil

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*Keywords*: *Mentha pulegium* L., essential oil, antioxidant activity, cholinesterase inhibition

The medicinal plant *Mentha pulegium* L. (Lamiaceae) is used in traditional medicine of Bosnia and Herzegovina to treat neurological and gastrointestinal disorders [1]. Healing properties of *M. pulegium* are attributed to monoterpenoids present in its essential oil and polyphenol derivatives [2]. These bioactive components have an important role in the prevention and treatment of chronic diseases related to oxidative stress. One of them is Alzheimer's disease, a neurological brain disorder and the most common form of dementia, affecting the older population. Inhibitors of cholinesterases have an important role in the treatment of Alzheimer's disease.
The aim of this work was to analyze the chemical composition as well as the antioxidant activity and cholinesterase inhibition potential of *M. pulegium* essential oil from Bosnia and Herzegovina. The chemical composition of the essential oil was determined by GC/MS and GC/FID techniques. The antioxidant potential was tested using DPPH and FRAP methods [3,4]. Inhibition of acetylcholinesterase and butyrylcholinesterase was determined using the Ellman's method [5]. The major components found in *M. pulegium* essential oil where: pulegone (54.4%; Fig. 1), *p*-menthone (14.0%), piperitenone (12.8%) and piperitone (3.7%). A solution of the essential oil (1 g/L) showed a low antioxidant potential and a good inhibition of both cholinesterases.

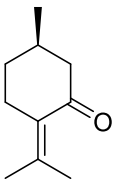


Fig. 1. (*R*)-(+)-Pulegone – the major compound found in *Mentha pulegium* L. essential oil

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# PP29. Essential oils from five *Nepeta* spp. cultivated in Lithuania and toxicological evaluation of their main components

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*Keywords*: *Nepeta* spp., essential oil composition, toxicological evaluation, hydrodistillation residues

The genus *Nepeta* (Lamiaceae) is widespread in central and southern Europe, Asia, the Middle East and North Africa; it has also been naturalized in North America and comprises about 300 perennial species [1]. *N. cataria* (catnip), which has been used for ornamental and culinary purposes and as a domestic folk-medicine remedy, is the most intensively studied among *Nepeta* species, [2]. Essential oils (EOs) of *Nepeta* spp. possess strong antimicrobial, antibacterial, antifungal, antiviral, anti-inflammatory, repellent and other activities [3,4]. The composition depends on the variety, growing site, climatic conditions, growth phase and analysis method. In general, the following main chemotypes can be distinguished: with nepetalactones, citral derivatives, 1,8-cineole and/or linalool as the dominant EO compounds [1,2]. Therefore, it was of interest to study the composition of EOs isolated from five *Nepeta* spp., namely *N. cataria* var. *citriodora*, *N. transcaucasica*, *N. melissifolia*, *N. sibirica* var. *citriodora* and *N. nuda* cultivated in Lithuania. It was determined that the yield of the hydrodistilled EO varied from 0.1 (*N. nuda*) to 0.6% (*N. cataria* var. *citriodora*). More than 140 volatiles were identified in the studied *Nepeta* spp. by GC-FID and GC×GC-TOF/MS. *N. cataria* var. *citriodora* and *N. nuda* may be characterized by 4aα,7α,7aα- and 4aα,7α,7aβ-nepetalactones, while *N. melissifolia* and *N. sibirica* var. *citriodora* contained large percentages of 1,8-cineole and caryophyllene oxide. The composition of *N. transcaucasica* was more complex and the oil contained citronellol, 4aα,7α,7aα- and 4aα,7α,7aβ-nepetalactones, geranial, neral, geraniol, 1,8-cineole and caryophyllene oxide as the major components. The toxicology of the main identified EO components was reviewed based on the previously reported data. In the second part of this study acetone extracts (using the solid phase obtained after hydrodistillation) and water extracts (liquid phase after hydrodistillation) from *Nepeta* spp. were prepared and evaluated for their antioxidant activities and total phenolics content in order to reveal the possibility of using *Nepeta* plants as a source of various functional food ingredients.

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## PP30. Hydrodistillation versus microwave-assisted hydrodistillation of sage herbal dust: kinetics, chemical profile and bioactivity

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*Keywords*: sage herbal dust, microwave-assisted hydrodistillation, kinetics, essential oil, bioactivity

Essential oils are gaining attention from the academic and industrial communities due to numerous biological activities and a broad spectrum of applications. With the arrival of the "green era", there was a need to reduce the production of waste materials and to make better use of natural resources. Due to the ever-increasing market of functional foods, the search for new natural, bioactive components is a hot topic on which a lot of research effort is being focused currently and biorefinery has recently emerged as a promising approach which could lead towards a sustainable concept of production. Therefore, the aim of this work was the valorization of sage herbal dust which is being generated as a by-product from filter tea factories. Conventional hydrodistillation (HD) and microwave-assisted hydrodistillation (MWHD) were applied for the essential oil recovery. The influence of heating (205 and 410 W) and microwave irradiation (90, 180, 360, 600 and 800 W) power on distillation kinetics and the chemical profile of the essential oils was evaluated. Empirical mathematical models were used for the modeling of process kinetics. The chemical profile was evaluated by HPTLC and GC-MS and monoterpenes (camphor, α-thujone, and eucalyptol), sesquiterpenes (viridiflorol) and diterpene polyphenols (epirosmanol) were the most abundant compounds identified. The high antioxidant capacity of the obtained essential oils, determined by the DPPH assay, suggested that sage herbal dust could be successfully utilized as a raw material for essential oil recovery.

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# PP31. High efficiency microfabricated planar columns for analysis of real-world samples of essential oils and plant volatile fraction

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*Keywords*: in-field analysis, planar columns, essential oils, plant volatile fraction

Compact and miniaturized instrumentation has obvious benefits in terms of energy consumption, materials, and laboratory space and, at the same time offers the possibility of "in-field" applications. In view of a possible application of on-chip GC for the analyses of essential oils in-situ with the industrial production and the volatile fraction emitted from plants, this study evaluates the performance of a set of planar columns developed to analyze complex mixtures. In a previous study, the performances of 2-m planar columns statically coated with apolar (Sil5%-PH), polar (FFAP-EXT), and chiral (Et-β-CD) stationary phases were tested. The results were comparable to those of reference conventional NB columns, efficiency achieving a number of theoretical plates per meter (N/m) ranging from 5700 for Et-β-CD to 7200 for Sil5%-PH [1]. Plant and food volatile fractions are characterized by high complexity and usually consist of components within a widely extended range of volatility and polarity. A reliable chemical analysis, therefore, requires columns with a high separation power. One of the ways to deal with this issue successfully is to increase column length while keeping high efficiency and selectivity. A set of 5-m planar columns (60 x 80 µm; nominal $d_c$ 0.71 µm) coated with the same stationary phases as in the previous study was therefore developed. Column performances were tested by analyzing essential oils (peppermint, lavender, chamomile, rosemary, tea tree, and bergamot) and headspace of the same aromatic plants, as well as standard mixtures of related compounds. The results were compared to those obtained with the 2-m planar columns of the previous study taken as reference. The 5-m planar columns provide separations of the components of the investigated samples fully overlapping on the corresponding conventional NB column. Their chromatographic performances were highly satisfactory achieving efficiency higher than the previous ones with N/m reaching 9300 for the FFAP-EXT planar column, and significantly increasing the retention of highly volatile compounds, thereby providing a drastic increase of their separation power (i.e. peak capacity). These results show that 5-m planar columns can provide performances that make them able to satisfy all requirements for a reliable analysis of complex samples such as essential oils and plant volatile fractions.

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# PP32. From medicinal and aromatic plants to herbal teas: quantitative determination of volatile bioactive secondary metabolites

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*Keywords*: aromatic plants, herbal teas, volatile secondary metabolites

Aromatic plants are worldwide used for their attractive aroma characterized by several volatile components, some of them presenting relevant biological activities. One of the most popular uses of aromatic plants is for herbal teas, therefore quality control of both raw plant materials and herbal teas is mandatory to guarantee the effective and, mainly, safe use of the finished product. Quali- and quantitative analysis of herbal teas evaluate the concentration of key-markers responsible for aroma and biological activities thus assessing a safe use of an herbal tea containing components limited by law or for which EMA (European Medicinal Agency) gives a recommendation on the maximum quantities to be consumed [1].

One of the issues concerning the analysis of aqueous samples is their not full compatibility with conventional stationary phases; this drawback can induce stationary phase degradation or problems in stability of column performance. An appropriate sample preparation procedure should, therefore, be used. Several conventional extraction techniques (i.e. solvent extraction) are time-consuming and often require a large volume of solvent; on the contrary, solvent-free sample preparation techniques (i.e. Solid Phase Micro Extraction both in solution and in headspace modes) make possible a direct sampling of an herbal tea, by adopting a fully automatic approach (TAS: Total Analysis System). To bypass completely the sample preparation step and, therefore, to speed up quality control, a new generation of gas chromatography columns, coated with ionic liquid-based stationary phases (Watercol$^{TM}$), compatible with aqueous samples, have been recently introduced [2].

The present work is focused on the quantification of biologically active secondary metabolites (e.g. menthol, α- and β-thujone, estragole, etc.) present in several plants most commonly used for herbal teas (i.e. wormwood, peppermint, sage, fennel, aniseed). Both approaches gave comparable results, together with a high repeatability, linearity, and accuracy.

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## PP33. Adulterated essential oils: when the chemical composition compliance with the European Pharmacopoeia misleads

Stefano Acquadro[1], Barbara Sgorbini[1]*, Cecilia Cagliero[1], Arianna Marengo[1], Carlo Bicchi[1], *Patrizia Rubiolo*[1]

*Keywords*: essential oils, adulteration, quantitative analysis

Essential oils are complex mixtures of volatile and semivolatile compounds obtained by hydro-, steam- or dry-distillation or by a suitable mechanical process without heating (for *Citrus* fruits) of a plant or of some parts of it [1]. The number of controls required, not only in terms of quality and safety but also of their biological activity, is constantly increasing. Quality control mainly aims at revealing the presence of adulterations or at quantifying compounds limited by law and it is mainly devoted to the evaluation of the EO chemical composition, usually, in terms of percentage abundance of selected markers, to be compared to reference values reported in Pharmacopoeias or in international norms.

In general, adulteration consists of the addition of cheaper essential oils or of synthetic compounds. This adulteration can be detected through the determination of the normalized percent areas of selected markers and, for chiral components, of their enantiomeric ratio. On the other hand, if a vegetable-heavy oil is added to "dilute" the essential oils, the normalized percent area is no longer diagnostic and a true quantitative analysis is necessary, provided that a reference sample is available.

This study aims at verifying how the two above approaches (percentage abundance and true quantitation) can be of help to detect adulteration with vegetable oil of lavender and bergamot essential oils. The results confirm that true quantitation is mandatory to highlight adulteration with non-volatile oils providing that a reference sample is available.

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# PP34. Effect of the essential oil from *Cantinoa carpinifolia* (Benth.) Harley & J.F.B.Pastore on efflux of potassium ions from *Escherichia coli* and *Staphylococcus aureus* strains

Karen Caroline Camargo[1]*, Luiz Roberto Batista[1], *David Lee Nelson*[2], Rafaela Magalhães Brandão[1], Vanuzia Rodrigues Fernandes Ferreira[1], Jéssica Oliveira e Nogueira[1], Maria das Graças Cardoso[1]

*Keywords*: terpenes, phenylpropanoids, antibacterial activity

Essential oils are secondary metabolites synthesized from glucose via two basic precursors, terpenes and phenylpropanoids. These compounds present diverse biological activities that reflect the very role they play in plants [1]. One of the most important properties is the antibacterial activity, although there are still few studies regarding the mechanism of action. *Cantinoa carpinifolia* (Benth.) Harley & J.F.B.Pastore, popularly known as rosman, is a plant species belonging to the Lamiaceae family and whose use in popular medicine is described in the treatment of diseases such as colds, flu, and rheumatism [2]. The objectives of the present work were to extract the essential oil from *C. carpinifolia* and to evaluate its effect on the efflux of potassium ions from strains of *Escherichia coli* and *Staphylococcus aureus*. The essential oil was extracted by the hydrodistillation technique using a modified Clevenger apparatus. The effect of the essential oil on the potassium efflux of bacterial strains was determined by flame photometry [3]. The concentrations tested were 6.25 μL $mL^{-1}$ and 0.39 μL $mL^{-1}$ for *E. coli* and *S. aureus*, respectively. The cell membrane is a barrier between the external and internal environments of the cell, being permeable to the passage of electrolytes that are important for various cellular functions, such as $K^+$ ions. The leakage of these ions indicates that an increase in permeability or rupture of the cell membrane occurred, affecting the functioning of bacterial cell metabolism and causing lysis. There was no significant variation between the five evaluated times (0, 60, 135, 197 and 267 min) for either of the bacteria nor did the concentration of potassium ions differ statistically when the treatments containing the essential oil and the control (bacterial culture) were compared. These results suggest that the essential oil from *C. carpinifolia* did not influence the cell membrane permeabilities of *E. coli* and *S. aureus* to potassium ions because there was no increase in the concentration of this ion at the evaluated times.

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## PP35. Chelating effect of carvacrol and the oregano essential oil

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*Keywords*: *Origanun vulgare* L., volatile oils, preservatives, antioxidants

Essential oils are natural products obtained from parts of plants by means of steam distillation. They are also made by expression of citrus fruit pericarp [1]. Because they are a complex mixture of chemical components, they exert innumerable biological activities, such as antimicrobial, antiparasitic, antitumor, antioxidant, among others. Because of the public demand for products of natural origin in different segments of society, essential oils have gained space, mainly in the food industries, where natural preservatives are sought that can replace or be associated with the synthetic additives used. One of the desirable properties of preservatives is their ability to interact with metal ions, such as iron, by exerting a chelating effect to inhibit lipid oxidation reactions catalyzed by these ions [2]. The objective of the present work was to evaluate the chelating effect of oregano essential oil and its major constituent, carvacrol, by cyclic voltammetry. The essential oil was extracted by hydrodistillation over a period of 2 hours using a modified Clevenger apparatus and characterized by gas chromatography coupled to mass spectrometric and flame ionization detectors. For the determination of the chelating effect, an electrochemical cell containing 0.05 mol $L^{-1}$ of anhydrous $Na_2SO_4$ was used as the supporting electrolyte, and $FeSO_4{\cdot}5H_2O$ 0.00150 mol $L^{-1}$ was the source of ferrous ions. Three electrodes were employed: Ag/AgCl (saturated in KCl) electrode was the reference, a platinum wire was the auxiliary, and glassy carbon was the working electrode. The determination of the chelating effect was performed by calculating the variation of the height of the ferrous oxidation peak with the increase in the concentrations of carvacrol and the essential oil. The essential oil from oregano contained terpinen-4-ol, carvacrol, *trans*-sabinene hydrate and γ-terpinene as the principal constituents. A reduction in the ferrous anodic current of 99.5 and 89% after the addition of 500 μg $mL^{-1}$ of carvacrol and oregano oil, respectively, was observed, thus indicating the occurrence of a chelating effect of oregano essential oil and its constituent carvacrol.

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# PP36. Cones and essential-oil production in hop with different nitrogen levels in the south of Brazil

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*Keywords*: *Humulus lupulus* L., mineral nutrition, essential oil composition

Hop crop requires a substantial amount of nitrogen (N) to meet growth and quality of production. Despite the increase of hop cultivated areas in Brazil in the last years, there is scarce information about hop nutrient requirements for soils of different regions of the country. The main objective of this work was to evaluate the effect of nitrogen levels in hop-cone production and its essential-oil yield and composition in the south of Brazil during the first year of cultivation. The field experiment was carried out in completely randomized blocks by comparing five nitrogen doses (50, 100, 150, 200 and 250 kg $ha^{-1}$) to non-fertilized plants, with four replications, each one with six plants. Urea was used as the nitrogen source being applied 20 kg $ha^{-1}$ for the fertilized treatments at the moment of planting which was complemented with a second dose 30 days after planting. Essential oil samples were obtained by hydrodistillation for two hours and their components were identified and quantified by GC/MS. The highest cone number per plant was obtained when 100 or 150 kg N $ha^{-1}$ were applied (2,677,066 and 2,518,082 cones $ha^{-1}$, respectively). Plants fertilized with 100 kg N $ha^{-1}$ had the greatest biomass (dry matter, DM) production (219.1 kg DM $ha^{-1}$), but with no statistical difference compared to plants fertilized with 150 or 200 kg N $ha^{-1}$ (210.1 and 199.6 kg DM $ha^{-1}$, respectively). The cone essential-oil yield varied from 0.46 to 0.69% but no statistical differences were found comparing all treatments. The major constituents of the essential-oil samples were myrcene (35.1-56.7%), (*E*)-β-farnesene (14.9-22.9%), β-selinene (6.6-11%), δ-selinene (7.2-12%), (*E*)-caryophyllene (3.5-2.6%) and linalool (0.28-0.47%). The results show that 100 kg N $ha^{-1}$ can be recommended for the first year of hop cultivation in the south of Brazil to obtain a greater cone number and biomass production with no effect on the essential-oil yield and composition.

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## PP37. Dermal application of oregano essential oil against recurrent urinary tract infections: an *in vivo* human pilot study

Meryem Özmen[1], Sanja Pavlović[1], Gerda Dorfinger[2,3], Karl Dorfinger[2], *Juergen Wanner*[4], Iris Stappen[1,3]*

*Keywords*: antimicrobial, SPME, human urine, bacteria count, thymol/carvacrol

Recurrent urinary tract infections, mainly affecting elderly women, drastically lower patients' quality of life. Furthermore, these persons are confronted with repeated intake of antibiotics (AB). Due to its high amount of phenolic monoterpenes thymol and carvacrol, oregano essential oil is known for its good antimicrobial effect [1] and therefore is used in complementary medicine as well as in aromatherapy.

In this pilot study, the antimicrobial effect of oregano oil (OO) was investigated *in vivo* on 21 patients (two men) suffering from an acute urinary tract infection, diagnosed in the doctor's office. These patients were divided into three therapy-groups (à seven): group 1 was medicated with ibuprofen (for pain relief) plus OO (5% diluted in jojoba oil), group 2 with an AB plus OO, and group 3 with an AB plus pure jojoba oil as a control group. Patients were instructed to apply the oils (OO or control) to their lower abdomen for five minutes twice a day for seven days. Urine samples were collected on day 1 (in the doctor's office) and day 8 (end of therapy) and examined for bacterial growth, respectively. Additionally, the symptoms, as well as the health conditions of the patients, were evaluated by means of questionnaires on days 1 and 8. Urine samples were analyzed by GC-MS for the presence of free, as well as their bound, amount of thymol/carvacrol by SPME. Group statistics were performed by ANOVA and t-tests.

Analyses of bacteria counts did not show any statistically significant differences between the therapies. In all three groups, bacterial growth was reduced, as well as health problems, on day 8 compared to day 1. This could be due to different infecting microbes, age differences between patients as well as probable additional over-the-counter medication (e.g. cranberry). Individual analyses suggested interesting findings which might be in relation to patients' body mass index (BMI). This should be complemented by GC-MS analyses which are still ongoing. These results will additionally be presented.

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# PP38. Comparison of hydrodistillation (HD), microwave-assisted hydrodistillation (MHD) and supercritical fluid extraction (SFE) for the isolation of volatiles from chamomile flower

*Jelena Arsenijević*[1]*, Aleksandra Cvetanović[2], Branimir Pavlović[2], Slavica Ražić[3], Zoran Maksimović[1], Zoran Zeković[2]

*Keywords*: *Matricariae flos*, essential oil, extract, bisabolol oxide, spiroether, azulene, sesquiterpene lactone

Chamomile flower (*Matricariae flos*) is a herbal drug used mainly because of antiphlogistic, spasmolytic and antimicrobial properties, which are related to the presence of volatile essential-oil constituents ($\alpha$-bisabolol and its oxides, chamazulene, spiroethers) and non-volatile compounds, such as sesquiterpene lactones, flavonoids, and coumarins.

In the present work, we used hydrodistillation (HD; sample-to-solvent ratio 1:20, 2 h), microwave-assisted HD (MHD; sample-to-solvent ratio 1:20, 2 h, microwave power 180 W) and supercritical $CO_2$ extraction (SFE; 40 °C, 100 bar, 3 h) to obtain isolates, from a commercially available chamomile flower tea. The composition of the isolates was analyzed using GC-MS. The obtained results of the relative content of the selected pharmacologically relevant constituents were as follows.

HD and MHD yielded 0.2% and 0.3% of isolates, respectively. A much higher yield was obtained in the case of SFE (3%). In HD and MHD isolates, which were qualitatively and quantitatively similar, oxygenated sesquiterpenes dominated (64.4-67.4%), with bisabolol oxides comprising 54.2-54.4% of the isolates. Among non-terpene constituents (17.0-19.9%), spiroethers were present with 10.0% and 11.7% of HD and MHD isolates, respectively. Chamazulene (4.8-4.9%) was the most abundant among sesquiterpene hydrocarbons (8.8-9.7%). On the other hand, non-terpene compounds (57.4%) were the most abundant class of constituents in SFE extract, and among them hydrocarbons comprised 45.0% of the extract, followed by 10.2% of spiroethers. Among the oxygenated sesquiterpenes (32.2%), SFE extract contained 25.8% of bisabolol oxides. In contrast to HD and MHD, SFE resulted in a low amount of chamazulene, but the extract contained 3.2% of valuable sesquiterpene lactones.

Having in mind that HD and MHD resulted in similar yields and compositions of the isolates, and that SFE gave a higher amount of the isolate with a unique composition, the choice of traditional vs modern technique for the preparation of chamomile isolates should be strongly dependent on the specific use of the final product and in that sense carefully evaluated.

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## PP39. Microbial growth inhibition by oximes derived from natural volatile carbonyl compounds

Alicja Surowiak[1], Agnieszka Dudek[1], Stanisław Lochyński[1,2], *Daniel Jan Strub*[1]*

*Keywords*: oximes, antimicrobial activity

Drug resistance rates in healthcare and community systems are induced by some bacterial and fungal pathogens. The answer to the challenge of antimicrobial resistance is searching for new alternatives to antibiotics.

The aim of our work was to evaluate the antimicrobial activity of low-molecular oximes, which have not been extensively studied with regard to this issue. Fifty-three oximes were screened *in vitro* for their growth inhibitory activity against seven strains of microorganisms: *Escherichia coli* (ATCC 10536), *Staphylococcus aureus* (ATCC 6538), *Enterococcus hirae* (ATCC 10541), *Pseudomonas aeruginosa* (ATCC 15442), *Legionella pneumophila* (ATCC 33152), *Aspergillus brasiliensis* (ATCC 16404), and *Candida albicans* (ATCC 10231). The growth inhibition of microorganisms was tested using the paper disc diffusion method. Three antibiotics, netilmicin, fluconazole, and ofloxacin, were used as reference controls for the tested microorganisms. The oximes' antimicrobial activity was evaluated by measuring the diameters of the inhibitory zones. Oximes of *trans*-cinnamaldehyde, propiophenone, (±)-citronellal, and piperitone showed strong antifungal activity, while the oximes of α-hexyl cinnamaldehyde, hydroxycinnamaldehyde, α-isomethyl ionone, pseudoionone, (-)-fenchone, and (+)-fenchone oximes showed strong antibacterial activity.

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## PP40. The analyses of commercial tea tree oils

*Jelena Radović*[1], Ivana Perišić[1], Tatjana Kundaković[1]*

*Keywords*: *Melaleuca alternifolia*, essential oil, terpinen-4-ol

Tea tree oil, the essential oil derived mainly from the Australian native plant *Melaleuca alternifolia* L. (Myrtaceae) is widely used as the active ingredient in many topical formulations for its antimicrobial activity, acting against viruses, bacteria, and fungi. Clinical studies have shown that this essential oil is very effective in various skin conditions, including acne, but also as an antiseptic in dentistry [1,2]. Since tea tree oil is commonly used, the aim of this study was to investigate the composition and quality of the three bestselling commercial tea tree oils in the Republic of Serbia, using GC and GC-MS analyses. All three oils had an almost identical composition. Among 42 quantified volatile substances, the most abundant in all samples were the oxygenated monoterpenes (46%), monoterpene hydrocarbons (45%), sesquiterpene hydrocarbons (6%), and oxygenated sesquiterpenes (1.5%). The major constituents are terpinen-4-ol (39.2%), γ-terpinene (17.6%), α-terpinene (7.4%), *p*-cymene (6.4%), limonene (4.3%), 1,8-cineol (3.7%), terpinolene (3.5%), α-pinene (3.2%), α-terpineol (2.8%), aromadendrene (0.9%), and sabinene (0.2%). The contents of all major components were within the range required by Ph. Eur. 9.0. In addition, all samples were tested for their quality based on measuring specific physical-chemical parameters (relative density, refractive index, and optical rotation) using suitable methods according to Ph. Eur. 9.0. Thus, it can be concluded that the tested samples of tea tree oil available on our market are of adequate pharmacopoeial quality.

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## PP41. The composition of the essential oils of *Acorus calamus* L. rhizomes from different habitats

Mirjana Marčetić[1], Slađana Škobić[2], *Jelena Radović*[1], Nikola Bošković[1], Anđela Damjanović[1], Tatjana Kundaković[1]*, Jovan Crnobarac[3]

*Keywords*: *Acorus calamus*, essential oil, β-asarone

Sweet flag rhizome (*Acorus calamus* L., Acoraceae) possesses various biological activities such as sedative, anticonvulsant, immunosuppressant, antidiabetic, antiinflammatory etc. [1]. The aim was to study the content and composition of essential oils from 24 rhizome samples of the cultivated sweet flag, their comparison with the samples from 5 natural habitats, and the influence of nitrogen fertilization on the composition of essential oils. Essential oils were analyzed using GC and GC/MS. Statistical analysis included the analysis of variance and cluster analysis. The content of essential oil was not significantly different between the samples from natural habitats (0.8-1.1%) and cultures (0.3-2.2%). All samples contained dominant oxygenated sesquiterpenes (24.5-32.6%), phenylpropanoids (5.7-22.5%), and oxygenated monoterpenes (4.4-19.2%). The main components were β-asarone (10.4-21.4%), camphor (3.5-15.2%), acorenone (9.3-14.1%) and cyperotudone (7.3-11.0%). The contents of β-asarone and aristolone were significantly higher ($p<0.05$) in cultivated plants. The nitrogen fertilization during the cultivation did not have a significant influence ($p<0.05$) on the content and composition of the essential oils.

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# PP42. Metabolism of essential-oil constituents: Determination of methyl and isopropyl *N*-methylanthranilates and their metabolites in rat organs

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*Keywords*: *Choisya ternata* Kunth, methyl and isopropyl *N*-methylanthranilates, metabolism, organs

Two volatile alkaloids, methyl *N*-methylanthranilate (MMA) and isopropyl *N*-methylanthranilate (IMA), identified in the essential oil of *Choisya ternata* Kunth (Rutaceae) [1], have been proven to possess diverse pharmacological activities, including antinociceptive, anti-inflammatory, gastro-, hepato- and nephroprotective activities, anxiolytic and antidepressant properties, as well as an effect on diazepam-induced sleep [2]. Recently, we investigated their urinary metabolite profiles [2]. However, their distribution in rat organs remained unknown. Herein we report on the identification and quantification of MMA, IMA and their metabolites in the organs (liver, kidney, heart, lungs, thigh muscle, and spleen) and serum of rats treated with these two substances (2 g/kg, *i.p.*). Diethyl-ether extracts of the serum and tissue homogenates were analyzed by GC and GC-MS. The largest amounts of both *N*-methylanthranilic acid esters' metabolites were found in the liver, while the lowest ones were found in muscles and spleen tissue. In the case of MMA, anthranilic acid and *N*-methylanthranilic acid were the major liver metabolites, while unmetabolized MMA was present in the liver in minute quantities. On the other hand, unmetabolized IMA was the predominant anthranilate derivative found in the liver, followed by *N*-methylanthranilic acid. Hydroxylated derivatives of MMA and IMA, were present in organ homogenates only in traces, probably due to their (easier) excretion via urine.

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## PP43. Volatiles from seven truffle species (*Tuber* spp.) wild-growing in Greece

*Eleni Stavraki*[1]*, Konstantia Graikou[1], Ioanna Chinou[1]

*Keywords*: *Tuber* spp., Greece, HS-SPME, phenolic content

In the framework of our phytochemical studies on mushrooms, we report herein, our analyses of seven selected species of *Tuber* (*T. aestivum, T. melanosporum, T. mesentericum, T. magnatum, T. borchii, T. brumale* and *T. uncinatum*), wild-growing in Northern Greece. Truffles are the fruiting bodies of mycorrhizal filamentous fungi well-known and part of the human diet, since antiquity [1] due to their unique and peculiar aroma. The aim of this study was to qualify and semi-quantify their aroma profile, as well as, to evaluate their total phenolic content, to the best of our knowledge for the first time on Greek truffles. The volatile organic compounds (VOCs) were analyzed by Headspace Solid-Phase Microextraction (HS-SPME) with two different polarity fibers (PDMS and CAR-PDMS) and led to the identification of more than fifty (50) VOCs. *T. magnatum*'s profile was characterized by aldehydes and other secondary metabolites, including its marker compound 2,4-dithiapentane [2]. In addition to this, amines and other nitrogen-containing derivatives were identified, leading to a distinction between the studied species. *T. mesentericum* was dominated by aromatic compounds, such as 3-methylanisole, previously referred to as its most characteristic chemical marker [3]. *T. melanosporum* and *T. brumale* were mainly characterized by aldehydes and *T. uncinatum, T. aestivum* and *T. borchii* showed an abundant presence of ketones and alcohols. Differing from all other studied samples, *T. borchii* was shown to emit the highest concentration of sulfur-containing derivatives, in accordance with the existing literature [4]. Moreover, all studied truffles were evaluated regarding their total phenolic content; *T. mesentericum* and *T. borchii* were the richest sources of phenolics (7.8 and 7.4 mg GAE (gallic acid equivalents)/g of the samples, respectively), followed by *T. aestivum* > *T. uncinatum* > *T. melanosporum* > *T. magnatum* > *T. brumale*.

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# PP44. The composition and antimicrobial activity of the essential oil of *Salvia officinalis* subsp. *oxyodon* (Webb & Heldr.) Reales, D.Rivera & Obón cultivated in the region of Murcia (Spain)

*Mariá José Jordán*[1]*, J. A Sotomayor[1], P. Sánchez-Gómez[2], I. García[1], P. Romero[1], M. Quílez[1], C. Martínez-Conesa[1]

*Keywords*: *Salvia officinalis* subsp. *oxyodon*, essential oil, antimicrobial activity

The aerial parts of Spanish sage (*Salvia officinalis* subsp. *oxyodon* (Webb & Heldr.) Reales, D.Rivera & Obón, Lamiaceae) have been used in the traditional Mediterranean medicine for its analgesic, antioxidant, sedative and antiseptic activities since ancient times. The main goal of the present work was to evaluate the bacterial growth inhibition curves of ten *S. officinalis* subsp. *oxyodon* essential-oil chemotypes, containing varying relative concentrations of secondary metabolites, against *Shigella sonnei* CECT 413, *Escherichia coli* CECT 45, *Salmonella enterica* subsp. *enterica* CECT 443, and *Listeria monocytogenes* CECT 911. A total of 30 individual plants (3 per chemotype) were used in this assay. The essential oils were extracted by hydrodistillation and the qualitative and quantitative composition was analyzed by a gas chromatograph coupled to a mass spectrometer (GC-MS). Among the total of 65 cultivated plants, collected in an experimental plot of land (Murcia, Spain), it was possible to identify the presence of 10 different chemotypes, based on the chemical composition of their essential oils. The majority of the plants belonged to a single chemotype, represented by eucalyptol and camphor. The inhibition growth curves were monitored for 48 h and the essential-oil concentrations ranged from 625 to 40000 ppm. The essential-oil chemical variability could be represented by the following chemotypes: eucalyptol (22-25%) and camphor (17-40%); camphor (40%) and eucalyptol (28%); camphor (37%), eucalyptol (8%), and α-pinene (11%); camphor (28%), eucalyptol (19%), and α-terpinyl acetate (18%); eucalyptol (22%), myrtenyl acetate (22%), and camphor (18%); camphor (37%), myrtenyl acetate (20%), and eucalyptol (7%); camphor (40%) and myrtenyl acetate (20%); linalyl acetate (21%), camphor (20%), and eucalyptol (18%).

From the results it can be concluded, that among the chemotypes studied, the ones containing 40-37% of camphor and 20% of myrtenyl acetate, at a concentration of 5000 ppm, was the most effective against *Shigella* and *Salmonella* (48 h) strains, while at a concentration of 20000 ppm, against *E. coli* (48 h) and *Listeria* (24 h) strains.

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# PP45. Antimicrobial activity and chemical variability of the essential oil of *Thymus hyemalis* Lange cultivated in the region of Murcia (Spain)

*Mariá José Jordán*[1]*, J. A Sotomayor[1], P. Sánchez-Gómez[2], I. García[1], P. Romero[1], M. Quílez[1], C. Martínez-Conesa[1]

*Keywords*: *Thymus hyemalis*, essential oil, antimicrobial activity

*Thymus hyemalis* Lange (Lamiaceae), winter thyme, is an endemic shrub growing on the Southeastern Iberian Peninsula, mainly in Alicante, Murcia, and Almeria. The main goal of the present work was to evaluate the chemical variability of the essential oils from this species and their antimicrobial activity based on bacterial growth inhibition curves. The chemical variability of the essential oils from this species was analyzed by means of gas chromatography-mass spectrometry. The oils were assayed to evaluate their bacterial growth inhibition curves against *Escherichia coli* CECT 45, *Salmonella enterica* subsp. *enterica* CECT 443, *Enterococcus faecalis* CECT 481, and *Listeria monocytogenes* CECT 911. Among the total of 53 cultivated plants, collected from an experimental plot of land in Torreblanca (Murcia, Spain), it was possible to identify the presence of eight different chemotypes, based on the chemical composition of their essential oils. The majority of the plants (53%) belonged to a phenolic chemotype, represented by a high content of thymol, and followed by *p*-cymene, eucalyptol, and carvacrol. The 48-h growth inhibition curves were obtained for the essential oil tested in concentrations that ranged from 156 to 5000 ppm. The essential-oil chemical variability was represented by the following chemotypes: (A) carvacrol (68%) and *p*-cymene (17%); (B) carvacrol (52%) and *p*-cymene (25%); (C) thymol (50%), *p*-cymene (25%), and γ-terpinene (10%); (D) *p*-cymene (44%) and thymol (41%); (E) *p*-cymene (41%) and thymol (30%); (F) *p*-cymene (40%) and carvacrol (33%); (G) eucalyptol (38%) and carvacrol (25%); (H) eucalyptol (38%) and thymol (22%). Besides, the essential oil yield ranged from 1.4 to 4.6%, showing statistically significant differences among the plants.

From these results it can be summarized that the chemotype C showed the highest effect against *S. enterica* (312 ppm), *E. faecalis* and *L. monocytogenes* (625 ppm), followed by the chemotypes with 60-50% of carvacrol, and then with 44% of *p*-cymene and 41% of thymol. The chemotypes with 38-30% of carvacrol, or thymol with *p*-cymene or eucalyptol did not inhibit the growth of *E. coli* and *S. enterica* (625 ppm), or of *L. monocytogenes* and *E. faecalis* (2500 ppm).

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## PP46. The isovalerate and 2-methylbutanoate of artemisia alcohol–new compounds from *Artemisia annua* L. essential oil

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*Keywords*: artemisia alcohol, libraries of compounds, esters

*Artemisia annua* L. (sweet wormwood) is an essential oil (EO)-rich, medicinally valuable plant species from the Asteraceae family [1]. During the analysis of the biologically active *A. annua* EO sample (hydrodistilled from the dry aboveground parts of the plants; oil yield 0.2%, w/w; the main components (relative abundance): artemisia ketone (35.7%), α-pinene (16.7%), 1,8-cineole (5.5%), artemisyl alcohol (4.8%), and *trans*-pinocarveol (4.8%) [1]), we have detected two minor compounds, AA1 and AA2 (0.06% and less than 0.05% of the total oil, with RI (DB5-MS) values of 1367 and 1373, respectively) with practically identical mass spectral (MS) fragmentation patterns (EI, 70 eV; *m/z* (rel. int.)): 169(15), 85(100), 57(38), 41(17). The comparison of GC (≈300 unit higher RI values) and MS data of AA1 and AA2 with those of artemisyl acetate (often present in EOs containing artemisia ketone and artemisia alcohol) suggested these might be esters of artemisia alcohol and (isomers of) pentanoic acids. To confirm this tentative identification, and possibly detect some additional AA1 and AA2 homologs, we prepared esters of artemisia alcohol and valeric, isovaleric, 2-methylbutanoic, butanoic, isobutanoic and propanoic acids (Steglich esterification; the starting alcohol was obtained by $LiAlH_4$ reduction of artemisia ketone isolated from the EO). Co-injection of the EO sample with synthetic standards confirmed AA1 and AA2 were artemisyl isovalerate and artemisyl 2-methylbutanoate (diastereomer not determined), respectively (Fig. 1). Detailed re-analysis of the EO revealed the presence of initially undetected trace amounts of artemisyl acetate. The results of this work once again confirm the importance of natural product-inspired libraries of synthetic compounds in the analysis of EOs, especially when it comes to the detection and identification of trace constituents.

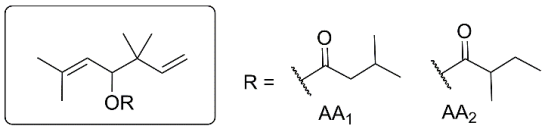


Fig. 1. Structures of artemisyl isovalerate (AA1) and artemisyl 2-methylbutanoate (AA2).

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# PP47. Odor of *ar*-turmerone, α-curcumene, and limonene derivatives depending on their chirality

*Toshio Hasegawa*[1]*, Yuka Hayakawa[1], Kenta Nakatani[1], Takeshi Tsuruoka[1]

*Keywords*: chirality, odor molecule, *ar*-turmerone, α-curcumene, limonene

The combination of many kinds of odor molecules produces the characteristic aromas of natural odor materials. We found that the odors of such materials were expressed by a set of constituents with similar structures by the investigations of the aroma profiles of several incenses [1]. Recent studies about the olfactory mechanism show that several olfactory receptors interact with one odorant molecule with different intensities and one olfactory receptor responds to different odorant molecules with similar structures. The consequences of this mechanism are that the interactions of several constituents with similar structures are important for the aroma profile. We investigated the relationship between odorant structure and the aroma characteristics of odor molecules focusing on their chirality.

Stereoisomers of *ar*-turmerone, α-curcumene, and limonene (Fig. 1) have been reported to have different odors. We synthesized a series of derivatives of these compounds to get insight into their structural similarities, especially those relating to the chirality and its interaction with olfactory receptors. We investigated the structure-odor relationships and found important structural factors (molecular skeleton, groups containing oxygen, isoprene moiety) for the onset of specific odors.

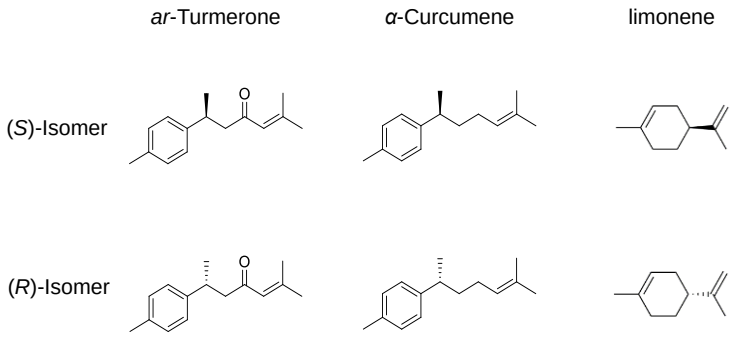


Fig. 1. Stereoisomers of *ar*-turmerone, α-curcumene, and limonene

*References*:

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# PP48. Essential-oil composition of parsley and celery conventionally and organically grown in Vojvodina

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*Keywords*: essential oil, chemical composition, parsley, celery

Celery (*Apium graveolens* L.) and parsley (*Petroselinum crispum* L.) are aromatic umbelliferous plants widely used as spices in the human diet due to the presence of essential oils. The chemical composition of the essential oils of aromatic plants can vary depending on the geographical origin, type of soil and agricultural practices [1,2].

In the present study, the influence of location (type of soil) and agricultural practices on the chemical composition of essential oils of parsley and celery leaf was investigated. The samples of both organically and conventionally grown plants were collected from different locations in the province of Vojvodina. The essential oil was isolated by hydrodistillation and then subjected to GC-MS analysis. Identification of chemical constituents was based on a comparison of their retention indices and mass spectra with spectral libraries and literature data. The main components of the essential oils obtained from parsley leaves were 1,3,8-menthatriene (22.8-50.9%), myristicin (12.8-36.8%), β-phellandrene (14.1-29.0%), and β-myrcene (1.4-12.7%). Celery leaf essential oils were mainly composed of β-phellandrene (41.7-72.6%), limonene (10.2-31.1%), and β-pinene (4.8-19.3%). The results obtained showed that there was no significant difference in the qualitative composition between the samples from different locations as well as between those grown in the conventional or organic way. On the other hand, the relative amount of particular compounds significantly varied between the samples in general, thus the correlation between their content and cultivation conditions or soil type could not be established.

In conclusion, the way of production has no specific effect on the qualitative composition of parsley and celery essential oils, although it can affect the relative quantity of their constituents.

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# PP49. Scents from the Brazilian Cerrado: The essential oil from *Siparuna brasiliensis* (Siparunaceae)

*Humberto R. Bizzo*[1]*, Marcelly C. S. Santos[1], Roberto F. Vieira[2], Rosa B. N. Alves[2], Ismael S. Gomes[2], Rafael F. Silva[3], Claudia M. Rezende[4]

*Keywords*: Brazilian biodiversity, Cerrado, *Siparuna*, cyclocolorenone

*Cerrado* is a term used to describe a savannah-like vegetation, occurring in Central Brazil. It is considered one of the 25 most important biodiversity hotspots in the world and has numerous herbs, including several aromatic plant families, many of which have never been subjected to chemical study [1]. *Siparuna brasiliensis* (Spreng.) A. DC. (family Siparunaceae) is an endemic Brazilian species, occurring in both the Cerrado and the Atlantic Forest [2]. Differently from other *Siparuna* species, very few chemical data are available about *S. brasiliensis*, and none so far regarding its essential oil. During a systematic investigation on the Cerrado flora, *S. brasiliensis* (CEN herbarium voucher 88294) was sampled in Brasilia, Brazil, and the essential oil obtained by hydrodistillation. According to Brazilian law, collection and access were authorized by the Ministry of Environment (process IBAMA 02001.003166/2013-26). The oil was analyzed by GC-FID and GC-MS on Agilent 7890A and 5975C systems, both with HP-5MS fused silica capillary columns (30 m x 0.25 mm x 0.25 μm). Oil components were identified by comparison of both mass spectra and linear retention indices with spectral libraries and literature. Oil yield was 0.7%. Only 11 compounds were detected, all but one identified by mass spectra and retention indices. Most of the constituents were closely related sesquiterpenes, with gurjunane and guaiane skeletons. The major compound was cyclocolorenone (75.5%). Other components present were 11-hydroxy-3,5-guaiadiene (tentative identification), 2-tridecanone (3.6%), α-cadinol (3.4%) and viridiflorol (3.4%).

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# PP50. Composition of the essential oil of the Balkan endemic *Thymus longedentatus* (Degen & Urum.) Ronniger

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*Keywords*: thyme, medicinal plant, aromatic plant

The genus *Thymus* comprises more than 250 species of perennial herbaceous or fruticose plants, classified into 8 sections. A total of 66 species with numerous subspecies and varieties are listed in the Flora Europaea. All species are considered important medicinal and aromatic plants. Twenty species grow spontaneously in Bulgaria. *Thymus longedentatus* is distributed only in the eastern part of the Balkan Peninsula (Bulgaria, Greece and Turkey), inhabiting sunny rocky habitats, mainly on limestone. Samples of this taxon were collected in the region of the Eastern Rhodopes. The essential oils were extracted from dried plant material by hydrodistillation using a Clevenger-type system and analyzed by gas chromatography coupled with mass spectrometry. The essential oils were characterized by a lemon-like odor due to the prevalence of citral isomers: neral (27.5%) and geranial (30.2%). Additionally, eucalyptol (7.8%), *trans*-β-ocimene (7.5%), germacrene D (4.4%) and β-myrcene (3.7%) were among other more abundant constituents of the oil. The remaining compounds were present in smaller percentage. Twenty-eight compounds comprising 98.2% of the total GC-areas detected were identified in the oil.

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## PP51. Organic vs conventional production of peppermint, lemon balm, and lavender; effect on yields and oil composition

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*Keywords*: essential oil crop, oil content, oil composition, organic production

Organic production and markets are expanding rapidly. A field study was conducted to compare effects of organic (OS) and conventional (CS) production systems and unfertilized control on peppermint (*Mentha x piperita* L.), lemon balm (*Melissa officinalis* L.), and lavender (*Lavandula angustifolia* Mill.) productivity and oil profile. *In peppermint*, both production systems provided greater yields than the yields in the unfertilized control. The application of vermicompost at 20 t/ha increased peppermint fresh biomass and essential oil yields with 20-31% and 24-28%, respectively, compared with the control. However, peppermint herbage and essential oil yields under OS were 7-87% and 13-54%, respectively, lower compared with the respective yields under CS. Overall, peppermint under OS had slightly higher essential oil content compared to the control; however, the oil composition was not significantly different from that in the CS. *In lemon balm*, fresh herbage yields in the OS were increased by 12-70% relative to the unfertilized control. However, compared with the yields at CS plots, yields in the OS were satisfactory only during the first year. In the second year, fresh herbage yields in the OS were up to 70% lower compared with those from the CS. The production system did not have a significant effect on the lemon balm oil content and composition. *In lavender*, the OS included two applications of probiotic product on six lavender genotypes. During the first year, CS lavender had 6 to 13% greater essential oil yield compared with the organically grown ones. In the second year, CS grown lavender out yielded OS grown by 9 to 24% in the case of inflorescence and 13 to 24% in the case of essential oil. However, during the third year of the study, the yields of inflorescences from OS stabilized and almost equaled those from CS. Overall, organic production of peppermint, lemon balm, and lavender may result in lower yields in the first 2-3 years, however, the essential oil content and composition may not be affected. Depending on the price premiums for organically produced herbage and essential oil, organically produced peppermint, lemon balm, and lavender may be economically and agronomically viable after the initial couple of years.

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# PP52. Scents from the Brazilian Cerrado: The essential oil from *Calea hymenolepis* (Asteraceae)

*Humberto R. Bizzo*[1]*, Marcelly C. S. Santos[1], Roberto F. Vieira[2], Rosa B. N. Alves[2], Ismael S. Gomes[2], Rafael F. Silva[3], Claudia M. Rezende[4]

*Keywords*: Brazilian biodiversity, Cerrado, *Calea*, α-phellandrene

The Brazilian Cerrado is a savannah-like biome with more than 12,000 botanical species in Central Brazil. It is an endangered biome, and considered to be a biodiversity hotspot [1]. *Calea hymenolepis* Baker is a shrub native from the Cerrado. Samples from a population (n>5) were collected from a rupestrian field in the Chapada dos Veadeiros National Park, in Goiás State, Brazil. According to Brazilian law, collection and access were authorized by the Ministry of Environment (process IBAMA 02001.003166/2013-26). A voucher was deposited at the Embrapa Genetic Resources herbarium and the essential oil was obtained from the leaves by hydrodistillation for 2 h, using a Clevenger-type apparatus. The oil was analyzed by GC-FID and GC-MS on Agilent 7890A and 5975C systems, both with HP-5MS fused silica capillary columns (30 m x 0.25 mm x 0.25 μm). Oil components were identified by comparison of both mass spectra and linear retention indices with spectral libraries and literature. Oil yield was 0.2%. Major compounds present were α-phellandrene (34.2%), *p*-cymene (10.6%), germacrene D (8.5%), (*E*)-β-caryophyllene (6.3%) and δ-elemene (4.6%). The oil composition was quite different from other *Calea*, like *C. clematidea*, rich in clematerol, a terpenic epoxide [3]. Although subject to systematic phytochemical studies since the 1980's, with the identification of sesquiterpene lactones, chromones, benzopyrans, flavonoids, chalcones and even acetylenes, very few studies have been published regarding the essential oil of *Calea* species [2]. To the best of our knowledge, this is the first analysis on the essential oil from *Calea hymenolepis*.

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## PP53. Brasilane sesquiterpenes, bioactive essential-oil constituents

*Sonja Filipović*[1]*, Niko Radulović[1]*

*Keywords*: brasilane, liverwort, volatile, biological activity

A bicyclo[4.3.0]nonane sesquiterpene skeleton with a *gem*-dimethyl group at C-3, methyl group at C-9 and an isopropyl group at C-5, is referred to as the brasilane skeleton. Biosynthetically, brasilanes originate from α-humulene. The structural complexity of this skeleton is illustrated by the first synthesis of conocephalenol from (1*R**,7a*S**)-1-methyl-7,7a-dihydroindan-5(6*H*)-one in 20 steps [1]. A shorter 7-step synthetic strategy was successfully accomplished by Cossy et al. starting from (*R*)-pulegone with an overall yield of 15% [2].

Up to now, 32 brasilane sesquiterpenes have been identified mainly in liverworts, fungi, and algae. Brasilane-type structures have been previously known only from marine organisms of the Rhodomelaceae family (species *Laurencia obtusa* (Huds.) Lamouroux and *Laurencia implicata* J.Agardh). In addition, brasilanes were detected in the sea hare *Aplysia brasiliana* due to its algae diet. A number of isolated derivatives bear an –OH at C-9, while there are four C-8 halogenated brasilanes and three metabolites with a 1,6-epoxy moiety [3]. In the equatorial liverwort species *Noteroclada confluens* (Hooker & Taylor) Spruce (Pelliaceae), two brasilane-type sesquiterpenes, similar to those found in *Conocephalum conicum* (L.) Dum. with tetrasubstituted double bonds at C-1, C-6, and C-5, were recorded. Xylarenic acid, possessing the brasilane structure, is recorded in the ascomycetous fungus *Xylaria* sp. [4]. The endophyte *Diaporthe* sp. [5], isolated from the leaves of *Rhizophora stylosa* Griff., yielded six brasilane-type sesquiterpenoids, diaporols J-O. *In vitro* cytotoxicity evaluation of brasilanes was performed on various human cancer cell lines (HL-60, SMMC-7712, A-549, MCF-7, HepG2, HCT116, MDA-MB-231, and SW480) [5,6]. A related, moderately cytotoxic, brasilane compound was isolated from the basidiomycete *Coltricia sideroides* (Lév.) Teng.

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# PP54. Juniper essential-oil composition and bioactivity as a function of species and sex

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*Keywords*: α-pinene; limonene; oxygenated hydrocarbons, sesquiterpenes

There are 10 species of juniper (*Juniperus* L., Cupressaceae) in the European flora, six of which (*J. communis, J. oxycedrus, J. pygmaea*, *J. sabina, J. sibirica*, and *J. excelsa*) are found in the Flora of Bulgaria. Of these, *J. excelsa* is monoecious and the other five species are dioecious. The objective of this study was to compare the essential oil (EO) composition, antioxidant, antimicrobial, and insecticidal activities of the male (M) and female (F) plants from the five dioecious species. A secondary objective was to compare extraction methods; Clevenger vs semi-commercial steam distillation on the EO yield, profile, and bioactivity of the juniper species. The concentration of α-pinene, β-caryophyllene, δ-cadinene, and δ-cadinol was different between the oils of M and F plants within all five species. Male and F plants of *J. pygmaea*, *J. sabina*, and *J. sibirica* had significantly different concentrations of sabinene within the respective species. In some cases, the EO of M and F plants had different antioxidant and antimicrobial activities. The extraction method, Clevenger vs semi-commercial steam distillation was also significant on the antioxidant capacity of the EOs within most juniper species. Overall, the EO obtained from the semi-commercial extraction was more consistent within a species with respect to antioxidant capacity compared with the oils obtained using the Clevenger-type extraction. However, the oils obtained via Clevenger extraction showed greater antioxidant capacity within a species compared with those from semi-commercial extraction. In two separate experiments, seven of the juniper oils (*J. communis*-F, *J. communis*-M, *J. oxycedrus*-M, *J. pygmaea*-F, *J. pygmaea*-M, *J. sibirica*-F, and *J. sibirica*-M) were tested for repellent and insecticidal activities against *Rhopalosiphum padi* (bird cherry-oat aphid) and *Sitobion avenae* (English grain aphid). All of the tested oils had significant repellent and insecticidal activities against the two aphid species at concentrations of the EO in the solution at 1%, 2.5%, and 5%. The results suggest that when reporting EO composition, antioxidant, antimicrobial, and insecticidal activity of juniper EO, the sex of the tree and the extraction method needs to be indicated along with the species. The results may benefit industry utilizing juniper leaf oil for new product development.

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## PP55. Analgesic activity of dehydrofukinone, a sesquiterpene ketone from *Senecio nemorensis* L. (Asteraceae)

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*Keywords*: *Senecio nemorensis* L., dehydrofukinone, analgesic activity

The genus *Senecio* is the largest genus of the Asteraceae plant family with more than 1500 species with a worldwide distribution [1]. In recent decades, the species of this genus have been extensively investigated for their secondary metabolites. It was shown that the genus is characterized by the presence of pyrrolizidine alkaloids and (furano)eremophilane sesquiterpenoids [1].

During a routine GC–MS screening of Asteraceae taxa from Serbia, it was found that the essential oil isolated from the aerial parts of *S. nemorensis* was dominated by a sesquiterpene ketone dehydrofukinone (75.1%). This eremophilane sesquiterpene was synthesized for the first time by dehydrogenation of fukinone isolated from *Petasites japonicum* Maxim in 1968 [2] and isolated a few years later from the leaves of *Arctium lappa* L. [3]. In the present work, this compound was isolated from the oil by column chromatography and assayed for its analgesic potential in animal models evaluating peripheral (abdominal writhing test) and central (hot plate and tail immersion tests) pain pathways. Prior to the experiments, group of animals were treated either with different doses of dehydrofukinone (50, 100 and 150 mg/kg), a standard drug (indomethacin/acetylsalicylic acid/morphine) or vehicle. The obtained results indicate that dehydrofukinone possesses moderate peripheral (at the highest dose) and mild central (only in the tail immersion test) analgesic activity. These findings are in agreement with previous publications which had also proven that *Senecio* sp. plant extract possesses only peripheral analgesic activity [4]. On the other hand *S. rufinervis* essential oil was found to significantly inhibit acetic acid-induced abdominal writhing in mice [5].

This plant species has proven to be a good natural source of this compound considering its high relative amount (about ¾ of the oil) and relatively high yield of the oil (0.12%, w/w of fresh plant material).

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# PP56. New natural products from *Clinopodium thymifolium* (Scop.) Kuntze (Lamiaceae) essential oil

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*Keywords*: *Clinopodium thymifolium*, *Micromeria thymifolia*, essential oil, new natural products

*Clinopodium thymifolium* (Scop.) Kuntze (syn. *Micromeria thymifolia* (Scop.) Fritsch) is an aromatic plant species widespread in the Mediterranean region, from north-eastern Italy across the Western Balkans to Hungary and Albania [1,2]. *C. thymifolium* has been used in folk medicine of the Mediterranean area for a long time [3]. Also, due to a high content of the essential oil in its leaves, it is used as a condiment and sometimes used in cooking [4,5]. For this reason, and the marked tendency to broaden the use of condiments and spices, some efforts are being made to introduce this plant as a new crop species (currently successfully cultivated in northern Italy) [4]. The beneficial effects of Lamiaceae species on human health have been frequently ascribed to essential-oil ingredients. Volatiles of *C. thymifolium* have been well studied – previous studies showed that the qualitative compositions of the investigated *C. thymifolium* oils were very mutually similar and dominated by oxygenated *p*-menthane monoterpenoids [6,7]. However, in this work, a comprehensive chemical analysis, in combination with detailed spectral analyses and chemical synthesis of selected compounds, has led to the identification of a series of esters of menthol stereoisomers in *C. thymifolium* essential oil, including some new natural products.

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# PP57. Oil yield and composition of *Juniperus oxycedrus* L. from Bulgaria and Serbia

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*Keywords*: α-pinene, limonene, oxygenated hydrocarbons, sesquiterpenes, *Juniperus deltoides*

*Juniperus oxycedrus* L. (Cupressaceae) is widely distributed in countries with a Mediterranean climate. The species is known for its large morphological and chemical variation and its debatable taxonomic status. The objective was to compare the essential oil content and composition of *J. oxycedrus* plants from Bulgaria and Serbia, and secondly, to quantify morphological variations of leaves. The essential oil content in dried juniper leaves varied from 0.059% (Kopaonik, Serbia) to 0.240% (Markovo, Bulgaria). Around 40 EO constituents were identified, belonging to the groups of monoterpenes, sesquiterpenes, diterpenes, and phenylpropanoids. The monoterpene hydrocarbons and oxygenated monoterpenes were the predominant groups of compounds representing 36.8-66.2% of the total oil, with α-pinene, limonene, sabinene, β-pinene, β-myrcene being the major constituents of this group. Overall, α-pinene was the major oil constituent in plants from all locations. The second largest group was the one of sesquiterpenes (sesquiterpene hydrocarbons, oxygenated sesquiterpenes), ranging from 19.3 to 33.6%. There was no significant difference between the mean leaf width of the six combinations of location and tree sex, and the overall mean width was 1.24 mm. However, there was a significant difference between the mean leaf lengths. This study contradicts recent reports that the European populations of *J. oxycedrus* east of Italy belong to a newly identified species *J. deltoides*. The same reports claimed that ”the leaf oil of *J. deltoides* was lower in α-pinene and higher in limonene compared to *J. oxycedrus”*. In this study, none of the studied populations had a higher concentration of limonene than that of α-pinene. Therefore, this study demonstrated that the flora of the two countries includes indeed *J. oxycedrus*.

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# PP58. The effect of steam distillation time on the yield and composition of the oil from *Kunzea ambigua*

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*Keywords*: *Kunzea ambigua*, steam distillation, essential oil, viridiflorol

*Kunzea ambigua* (Sm.) Druce (Myrtaceae), commonly known as 'Tick Bush' is a woody shrub, indigenous to Australia and New Zealand. It thrives in the granite soils of the north-east coast and Bass Strait islands of Tasmania. The therapeutic and antimicrobial properties of the essential oil have been documented [1,2]. The nature of the small, leathery leaves necessitates a long distillation time to achieve maximum oil yield. Oils were collected at set distillation times of 1, 3, 5, 10, 30, 60, 90, 120, 150, 180, and 240 mins. Yields and chemical compositions were determined by GC FID and identification of components was confirmed by Kovats Indices and mass spectra. Although the distillation of monoterpenes contributed to the most rapid phase of oil accumulation, which occurred at around 30 minutes, the narrow, lanceolate leaves of *K. ambigua* required in excess of 4 hours for complete extraction of the heavier components. The concentration of oxygenated monoterpenes, such as terpinen-4-ol and α-terpineol, had peak oil recovery at between 30 and 60 minutes. Recovery of 1,8-cineole maximized at 30 minutes, following a similar pattern to the monoterpenes. The cyclic ether component of this oxygenated monoterpene may well contribute to the different behavior under the conditions of steam distillation. In contrast, increasing amounts of the oxygenated sesquiterpenes, globulol and viridiflorol accumulated with time and it may be assumed that the complete extraction of essential oils from the vegetative material was not achieved. Both components are regarded as integral to the aroma, contributing a floral/citrus element to the bouquet of the typical *Kunzea* oil [3]. Oils containing higher ratios of these heavy components may be achieved by combining fractions collected onwards from one and a half hours into the steam distillation process. This enhanced the percentage of globulol from 17±3 in the unfractionated, total oil yield to 27±4 in the 46% of the oil collected in the later stages of the distillation. Likewise, the percentage of viridiflorol can be increased from 10±2 to 17±2%. Research is continuing into shortened distillation times using super-heated steam and into the antibacterial and antifungal properties of the oil of *K. ambigua*.

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## PP59. The effects of Scots pine (*Pinus sylvestris* L.) essential oil in an endotoxin-induced acute airway inflammation mouse model

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*Keywords*: Scots pine, essential oil, airway inflammation, LPS, mouse model

Inflammatory lung diseases affect a large population at every age worldwide. Essential oils (EOs) can easily reach the respiratory tract via inhalation due to their volatility. The antiinflammatory effect of EOs is poorly studied and there are only a few *in vivo* data. Therefore, we investigated the chemical composition and effects of Scots pine EO in the endotoxin-induced acute airway inflammation model in mice. The EO was selected on the basis of its potent antibacterial activity.

The chemical composition of the EO was determined by gas chromatography-mass spectrometry. Airway inflammation was evoked by 100 µg intratracheal endotoxin administration (*Escherichia coli* 083 lipopolysaccharide: LPS) to female C57BL/6 mice (n=8/group). There were three 30-min long inhalation sessions of the EO for during the 24-h period of the experiments. Airway function was measured by unrestrained whole-body plethysmography in conscious, awake animals. Myeloperoxidase (MPO) activity was determined by spectrophotometry from lung homogenates, while the semiquantitative histopathological score was evaluated from hematoxylin-eosin stained lung sections.

α-Pinene (39.4%) was the main component of the tested Scots pine oil. The inhalation of the EO significantly reduced peak inspiratory and expiratory flow and LPS-induced airway hyperresponsiveness compared to the paraffin oil-treated controls. Scots pine oil significantly reduced the perivascular edema formation. However, the EO significantly increased MPO activity. Scots pine oil or its components may be considered as a potential adjuvant in the treatment of respiratory symptoms.

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## PP60. Essential-oil component combinations: possibilities against respiratory tract pathogens

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*Keywords*: essential oil, interaction, respiratory infections, bacterial resistance, MRSA

Nowadays, the excessive use of antimicrobials leads to the growing appearance of resistant pathogens in the case of respiratory tract infections (RTIs). Therefore, the discovery of new alternatives, which could support their therapy is an important challenge. Combination of the effective substances is one of the possible solutions. Based on this possibility, several studies focused on the interaction between essential oils (EOs) and their volatiles in the last decade.

Therefore, the aim of the present study was to evaluate the most effective EO components of cinnamon bark, thyme, clove, peppermint, and citronella oils. Direct bioautography (DB) was used in the detection of interaction profiles of *trans*-cinnamaldehyde, eugenol, thymol, menthol, geraniol, citronellal, and citral against methicillin-resistant *Staphylococcus aureus* (MRSA, 4262), resistant *Pseudomonas aeruginosa* (RPA, 34205), and *P. aeruginosa* (ATCC 27853). First, the minimal detectable dose (MDD) of individual components was determined. According to the MDD values, the combined, as well as the individual compounds, were applied to the TLC plates. The diameters of the inhibition zones were measured with the Motic Images Plus 2.0 program. The statistical analysis was performed with the Mann-Whitney-Wilcoxon test of the R Studio 1.1.383 program.

In the case of *P. aeruginosa*, a combination of thymol and menthol was active; against RPA, *trans*-cinnamaldehyde combined with thymol was found to be effective. Against MRSA, menthol combined with *trans*-cinnamaldehyde, and eugenol also showed enhanced activity.

According to our knowledge, we applied for the first time the DB for the detection of antimicrobially effective combinations of EO compounds. It could be regarded as a cost-effective and quick screening method. In the future, we would like to focus on the combinations of EOs and their main components with antibiotics as well.

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## PP61. The effect of coriander essential oil on the oxidative stability of cooked pork sausages

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*Keywords*: *Coriandrum* essential oil, cooked pork sausage, oxidative stability, flavor

The effect of coriander essential oil (CEO) at concentrations of 0.075-0.150 µL/g on lipid oxidation (thiobarbituric acid reactive substances-TBARS method) and flavor of cooked pork sausages was investigated. CEO addition caused a statistically significant ($p<0.05$) decrease of TBARS values compared with the control, which can probably be accredited to the antioxidant potential of coriander essential oil. The addition of CEO in concentrations of 0.100 µL/g and 0.125 µL/g produced only slight differences in flavor. However, slight/moderate flavor differences were observed for sausages produced with 0.150 µL/g of CEO compared to the control ones. Hence, the obtained results showed that the addition of CEO in concentrations of 0.075-0.125 µL/g had no negative impact on the sensory properties of cooked pork sausages. Therefore, the results of this paper revealed the significant antioxidant activity of CEO, and consequently its high potential for utilization in the processing of cooked pork sausages. These results are encouraging with respect to an increasing demand for the use of essential oils as alternatives for synthetic antioxidants in meat processing.

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# PP62. *Satureja hortensis* L. essential oil causes *Acinetobacter baumannii* membrane disruption

*Verica Aleksić Sabo*[1]*, Neda Mimica-Dukić[2], Rok Kostanjšek[3], Jelena Narančić[1], Isidora Nikolić[1], Petar Knežević[1]

*Keywords*: essential oils, *Acinetobacter baumannii*, scanning electron microscopy, minimal inhibitory concentration, autoaggregation

Essential oils are promising antimicrobial agents against various bacteria, including *Acinetobacter baumannii*, a highly resistant clinical opportunistic pathogen with an increasing prevalence. The traditional application of the aromatic and medicinal plant *Satureja hortensis* L. (Lamiaceae) as a natural remedy for the treatment of inflammatory diseases, nausea, diarrhea, and various infectious diseases is well known. The aim of the study was to determine the antimicrobial activity and potential target site for *S. hortensis* essential oil against *A. baumannii*. The effect of the essential oil was determined using the microdilution broth method. The determined minimal inhibitory concentration (MIC=1 µl $mL^{-1}$) showed that *S. hortensis* essential oil possesses a significant anti-*A. baumannii* effect. The *A. baumannii* reference strain ATCC 19606 cells in the exponential growth phase were treated for 3 h at 37 °C with MIC of *S. hotensis* essential oil and examined by scanning electron microscopy. The electron micrographs highlighted the occurrence of collapsed cells with perforations, cell content leakage, cell debris, but also cell autoaggregation (Fig. 1B). The autoaggregation was further confirmed by an autoaggregation test: untreated cells (Fig. 1A) were partially autoaggregative, while the treated cells were highly autoaggregative, as a result of changes of the cell surface properties. Thus, the essential oil affected the membrane systems of *A. baumannii* cells, causing structural changes of the bacterial cells. Since *A. baumannii* strains are susceptible to *S. hortensis* essential oil, the oil possesses a great potential in the control of growth of this species.

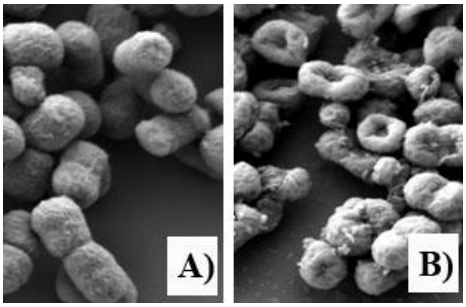


Fig. 1. *S. hortensis* essential oil effect (B) on the cells of *A. baumannii*; untreated control (A); magnification 20,000×

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## PP63. Composition and phytotoxic activity of the essential oils of two invasive plant species

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*Keywords*: allelopathy, biological activity, giant hogweed, GC-MS, small balsam

Alien species have been entering Europe for centuries. Their numbers have risen exponentially. Invasive species have multiple negative ecological, economic and human-health impacts. Chemicals produced by alien species are allelopathic to native species which are less resistant to them. This effect probably enables alien species to spread to new areas [1]. The possible use of natural compounds in weed management has been well documented [2,3].

Our research focused on two invasive species–*Heracleum mantegazzianum* Sommier et Levier (Apiaceae, giant hogweed) and *Impatiens parviflora* DC. (Balsaminaceae, small balsam). Giant hogweed produces a large number/amount of chemical compounds, such as coumarins and esters [4]. Many groups of active compounds have been isolated from different species of the genus *Impatiens* [5]. However, only few reports are available concerning the volatile constituents of both species.

The aim of the present experiment was to determine the quantitative and qualitative properties of the essential oils (EOs) hydrodistilled from the two invasive species. The phytotoxic effect was tested on selected dicotyledonous plant species. Different biological effects were evaluated in different concentrations of EOs.

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## PP64. Investigation of the potential influence of soil contamination on the phytotoxic activity of the essential oil from *Solidago canadensis* L.

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*Keywords*: *Solidago canadensis*, phytotoxic activity, soil contamination, heavy metals

*Solidago canadensis* L. (Asteraceae) is one of the most aggressive European plant invaders [1]. It has caused serious harm to crop production, orchards, lawns, natural environments and a loss of biodiversity [2]. Like most plants, this species also produces secondary metabolites, which are released into the environment. Scientists believe that these chemicals could be behind the success of their invasion [3]. Great progress has been made over the past decades in the study of chemical composition of *S. canadensis*. Dominant chemical components had been investigated as saponins [4], polyphenols, flavonoids, organic acids [5] and essential oils [6,7]. Also, its biological activities were studied [8-10].

The aim of the present research was to determine the level of phytotoxic effect of essential oil (EO) hydrodistilled from the *S. canadensis* from three localities with different soil contamination. Cd, Pb, Cr and Cu amount were determined to decrease with the distance from the source of contamination. The quantity of EO increased with the higher level of heavy metals in soil. Phytotoxic activity of EO was tested on seeds of two dicotyledonous plant species (*Raphanus sativus* L. and *Lepidium sativum* L.) and the different effect was observed depending on EO concentrations and model plant seeds.

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# PP65. Essential-oil composition of *Zygophyllum fabago* aerial parts from Turkey

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*Keywords*: essential oil, *Zygophyllum fabago*, phytol, (*E*)-β-damascenone, farnesyl acetone C

There are many reports in the literature, related to the essential oil of *Zygophyllum* species (Zygophyllaceae), but several reports describe the antioxidant activity of this genus. Previously, sesquiterpene hydrocarbons and diterpenoids were reported from *Zygophyllum fabago* L. as the main components [1]. Current research aims to provide information on the essential-oil composition of *Z. fabago* collected from Ankara, Turkey. The essential oil was obtained by hydrodistillation from air-dried aerial parts of the plant with a Clevenger apparatus for 3 h. The essential oil yield of the plant was in trace amount. The oil was recovered with *n*-hexane (1 mL) and dried over anhydrous $Na_2SO_4$. The essential oil was analyzed without further dilution and used in the GC-MS analysis. The essential oil was analyzed with an Agilent 5977 MSD GC-MS system operating in EI mode; injector and MS transfer line temperatures were set at 250 °C. Splitless injection was used in the analysis. Innowax FSC column (60 m x 0.25 mm, 0.25 µm film thickness) and helium as the carrier gas (1 mL/min) were used in GC-MS analyses. The oven temperature program was: 60 °C for 10 min and then raised to 220 °C at a rate of 4 °C/min, afterwards the temperature was kept constant at 220 °C for 10 min and then raised to 240 °C at a rate of 1 °C/min. Mass spectra were recorded at 70 eV with the mass range *m/z* 35-425. Relative amounts of the separated compounds were calculated from the integration of the peaks in MS chromatograms. Identification of essential-oil components was carried out by comparison of their retention indices (RI), relative to a series of *n*-alkanes ($C_5$ to $C_{30}$), with the literature values, as well as by mass spectral comparison. The aerial parts essential oil of *Z. fabago* yielded an essential oil rich in oxygenated monoterpenes and diterpenes. The major components of the essential oil were: (*E*)-phytol (11.7%), (*E*)-β-damascenone (10.1%), farnesyl acetone C (5.1%), dihydromethylionone (3.9%), (*E*)-geranyl acetone (3.7%), γ-decalactone (3.6%), (*E*)-β-ionone (3.3%), pentacosane (3.4%), hexahydrofarensyl acetone (2.5%), and hentriacontane (2.8%).

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# PP66. Chemical composition of the essential oil from the aboveground parts of *Santolina chamaecyparissus* L. from Greece: NMR determination of the exocyclic double bond geometry of the major spiroketal-enol ether polyynic constituent

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*Keywords*: *Santolina chamaecyparissus* L., essential oil, 2D NMR, stereochemistry, spiroketal-enol ether polyyne

*Santolina chamaecyparissus* L. (Asteraceae), commonly referred to as cotton lavender, is a semi-woody perennial plant with aromatic evergreen foliage, native to the Mediterranean area. Thus far, a number of researchers have analyzed the composition of the essential oil of this plant taxon, and these studies reveal a great variation in the content and identity of its volatile secondary metabolites. Herein we present a detailed GC-MS analysis of the essential oil obtained by hydrodistillation from the fresh aboveground parts of *S. chamaecyparissus* collected during winter time in Greece (central Macedonia). Fifty-four constituents were successfully identified from the small amount (0.325% yield) of the dark yellow essential oil, representing almost 97% of the total detected GC-peak areas. The main constituents of the essential oil were found to be artemisia ketone, vulgarone B, and 7-(2,4-hexadiynylidene)-1,6-dioxaspiro[4.4]nona-2,8-diene. The mass spectrum of the detected spiroketal-enol ether polyyne, along with an extensive literature research of RI values were not sufficiently informative to infer the exocyclic double bond geometry of this major constituent of the essential oil. However, a direct analysis of $^{1}$H- and $^{13}$C-NMR spectra (recorded at 400 MHz, in $CDCl_3$) of the essential oil combined with 2D NMR experiments (gradient $^{1}$H-$^{1}$H COSY, HMBC, and HSQC) enabled the full structural and stereochemical assignment. Additionally, the chemical shift of the enol ether proton (on the very double bond) was in an agreement with literature data [1] and we concluded that the compound in question was (*Z*)-7-(2,4-hexadiynylidene)-1,6-dioxaspiro[4.4]nona-2,8-diene. The comparison of mass spectra of the *Z*- and *E*- isomers (the latter was present in the oil with 0.85%) shows minor differences, which strongly indicates that the mass spectra alone would not be adequate for a reliable identification.

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# PP67. Identification and 2D NMR structural elucidation of a $C_{10}$-polyacetylenic ester, a previously unreported constituent of *Bellis perennis* L. essential oil

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*Keywords*: *Bellis perennis* L., polyacetylenic ester, structural elucidation, 2D NMR, matricaria ester

Common daisy, *Bellis perennis* L., is a widespread herbaceous perennial plant species from the Asteraceae family. Although it has a history of traditional use for the treatment of a variety of health conditions [1], up to now only a few studies dealt with the composition of the essential oil of this plant taxon [1]. Hydrodistillation of the fresh aboveground parts, collected at the beginning of anthesis from a wild-growing population in Serbia (Jelašnica gorge), yielded a small amount of a light green essential oil (0.022%), which was analyzed by GC-MS and a total of 33 compounds was identified (97.1%), with polyacetylenes as one of the major chemical classes detected. The essential oil was chromatographically separated on a 10% $AgNO_3$-coated silica column, which resulted in one polyacetylene-enriched fraction. GC-MS analysis of this fraction revealed the presence of two $C_{10}$ polyacetylenic compounds. One of them was identified as methyl deca-4,6-diynoate (2,8-tetrahydromatricaria ester), previously reported [1] as one of the main polyacetylenes present in the essential oil of *B. perennis*. Literature data [1] and the mass spectrum of the other polyacetylenic compound, present in the oil in trace amount, suggested that it was likely to be a lachnophyllum ester (8,9-dihydromatricaria ester). Direct analysis of $^{1}$H- and $^{13}$C-NMR (at 400 MHz, in $CDCl_3$) spectra of the obtained fraction proved to be challenging, due to signal overlap. However, a combination of 2D NMR experiments (gradient $^{1}$H-$^{1}$H COSY, HMBC, and HSQC) enabled a full structural assignment. The compound in question was demonstrated to be methyl (*Z*)-deca-8-en-4,6-diynoate (i.e. a 2,3-dihydromatricaria ester), which, to the best of our knowledge, has not been reported in *B. perennis* until now. It is possible that the previous reports [1] of lachnophyllum esters in common daisy essential oil, based solely on MS data, are in fact incorrect due to minor differences in the mass spectra of the isomeric esters.

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## PP68. Antioxidant activity of lemongrass essential oil and its constituents

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*Keywords*: *Cymbopogon citratus*, functional food, antioxidant activity

Plants and their ingredients (essential oil, flavonoids, etc.) are considered to be functional food if specific health benefits are attained by their consumption. These benefits include mostly preventive and protective but sometimes curative properties against one or more diseases, usually the so-called civilization diseases (different types of cancer, cardiovascular and neurodegenerative diseases) [1]. The essential oil (EO) obtained from *Cymbopogon citratus* (DC.) Stapf. (Poaceae) is a perfect functional food ingredient. Its characteristic, pleasant and refreshing odor goes hand in hand with its antiinflammatory, diuretic and sedative activities, due to which the plant was used in folk medicine for the treatment of nervous and gastrointestinal illnesses [2].

The aim of this work was an assessment of the antioxidant activity of lemongrass essential oil and its constituents. EO was hydrodistilled from the leaves and also the stems of *C. citratus* grown in Poland, while its chemical composition was analyzed by GC-MS. Both essential oils had a very similar chemical composition, with the exception of the presence of a sesquiterpene alcohol, elemol, in the stems oil, as well as a different antioxidant activity, which was higher for the EO obtained from the stems. The next stage of our research work was the isolation of the major components by the use of high-performance counter-current chromatography (HPCCC). The isolated compounds, neral, geranial, and elemol, as well as citronellol and citronellal, were subjected to antioxidant activity testing by TLC-bioautography using DPPH as the detection reagent, as well as by the CUPRAC method. However, the performed studies did not confirm the antioxidant activity of the major components alone present in the lemongrass essential oil. In total, neral, geranial, and elemol constituted 84.2% of all components present in the EO from *C. citratus* stems but they were not responsible for the observed antioxidant effect. It can be concluded that the antioxidant activity of lemongrass oil is the result of a synergistic effect of all ingredients present in this EO.

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## PP69. The nanotechnological formulation and anti-biofilm activity of thyme essential oil against *Streptococcus pneumoniae*

Viktória L. Balázs[1]*, Barbara Horváth[2], Erika Kerekes[3], Aleksander Széchenyi[2], Adorján Varga[4], Béla Kocsis[4], *Kamilla Ács*[1], Judit Krisch[5], Györgyi Horváth[1]*

*Keywords*: thyme oil, Pickering-emulsion, *S. pneumoniae*, anti-biofilm activity

Bacterial biofilm is a structured community of bacterial cells enclosed in a self-produced polymeric matrix and adherent to an inert or living surface, which allows a protected mode of growth and survival in a hostile environment. Infections associated with biofilm growth usually are challenging to eradicate. It is mostly due to the fact that mature biofilms display tolerance towards antibiotics and the immune response. For example, bacterial biofilms can be formed in the human respiratory tract. The essential oil of thyme (*Thymus vulgaris* L., Lamiaceae) is well-known in the therapy of respiratory tract infections, but there is no information about the anti-biofilm activity of its hydrophilic formulation against respiratory tract pathogens.

The aim of the study was to investigate the anti-biofilm effect of a thyme oil (Aromax Ltd., Hungary) formulated with nanotechnology against *Streptococcus pneumoniae* (DSM 20566). The oil was analyzed by GC-FID/MS. The Pickering emulsion of the oil was produced via the Stöber synthesis and stabilized with silica-nanoparticles. The bacterial biofilm ($10^8$ CFU/mL) was created in 96-well microtiter plates. After incubation (4 h, 37 °C), the Pickering emulsion and the Tween 80 solution of the thyme oil were added to the biofilm in MIC/2 concentration (0.05 mg/mL). After a second incubation (24 h), the adherent cells were fixed with methanol and stained with 0.1% crystal violet and dissolved in 33% acetic acid. The absorbance (A) was measured at 590 nm with a plate reader (BMG Labtech).

Our results showed that the thyme oil had anti-biofilm activity against *S. pneumoniae*, because it reduced the biomass of the biofilms. It is important to highlight that the Pickering emulsion of the oil was more effective (A = 0.53) than the Tween 80 solution (A = 0.84) compared to the control (A = 3.71). This confirms that the Pickering emulsion of thyme oil can prevent the *S. pneumoniae* biofilm formation more effectively than the Tween 80 solution.

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## PP70. Volatile compounds from different species of *Lycopodium* with anti-tuberculosis activity

*Aleksandra Dymek*[1]*, Jarosław Widelski[1], Joanna Golus[2], Gabriela Widelska[3], Rafał Sawicki[2], Grażyna Ginalska[2], Krystyna Skalicka-Woźniak[1], Tomasz Mroczek[1]

*Keywords*: *Lycopodium*, *Mycobacterium tuberculosis*, H37Ra

Different species belonging to the genus *Lycopodium* L. (Lycopodiaceae) were used in folk medicine due to their antibacterial, healing effects on wounds, and properties used in the treatment of mental diseases, like amnesia, schizophrenia and different types of dementia.

Extracts containing volatiles obtained from different *Lycopodium* species: *L. clavatum*, *L. annotinum*, and *Huperzia serrata* (syn. *Lycopodium serratum* Thunb.), were tested against *Mycobacterium tuberculosis*. Dichloromethane and petroleum ether extracts of the mentioned species collected in different geographical sites (in Poland and Ukraine) have shown interesting activities.

Minimal Inhibitory Concentrations (MIC) values for the extracts were determined by a 96-well microplate method with alamarBlue (Invitrogen). The inoculum of the reference strain of *Mycobacterium tuberculosis* H37Ra in Middlebrook 7H9 broth (Difco) was 5 x $10^5$ cfu/mL per well, according to CLSI standards. Serial twofold dilutions of the extracts ranged from 8 to 256 µg/mL. As the internal control of the method, serial twofold dilutions of four first-line antibiotics dedicated to tuberculosis treatment: isoniazid (INH), rifampicin (RMP), ethambutol (EMB), and streptomycin (SM) were used [1,2].

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## PP71. GC-MS analysis of volatiles from different *Lycopodium* species with acetylcholinesterase activity

*Aleksandra Dymek*[1]*, Jarosław Widelski[1], Agnieszka Ludwiczuk[1], Krystyna Skalicka-Woźniak[1], Tomasz Mroczek[1]

*Keywords*: *Lycopodium*, GC-MS, acetylcholinesterase inhibitors

Searching for natural inhibitors of different enzymes, e.g. acetylcholinesterase (AChE), is a modern approach in drug discovery. *Lycopodium* L. (Lycopodiaceae) species containing alkaloids appear to be a rich source of acetylcholinesterase inhibitors.

In our study, a GC-MS analysis of the extracts of *L. clavatum*, *L. annotinum*, and *Huperzia serrata* (syn. *Lycopodium serratum* Thunb.), containing volatile constituents with AChE-inhibitory activity, was performed. The detection of AChE-inhibitory activity of the investigated extracts was achieved by TLC-bioautography.

The GC-MS analysis was carried out on a Shimadzu GC-2010 Plus chromatograph coupled to a QP2010 Ultra mass spectrometric detector using a Phenomenex capillary column ZB-5MS (30 m; diameter of 0.25 mm and thickness of 0.25 µm). The initial column temperature was set to 50 °C, which was held for 3 min, and in the next step, the column was heated to 250 °C at a rate of 8 °C per min (and was then held at that temperature for 2 min). The split ratio after the injection of 1 µL was 1:20 and helium was used as the carrier gas (the flow rate was 1 mL per min). Ionization was performed by electron impact at 70 eV. The identification of compounds was based on a comparison of their mass spectra with those of MassFinder and NIST mass spectral libraries, as well as by retention index (calculated based on a homologous series of *n*-alkanes) comparison.

The GC-MS analysis allowed the identification of alkaloids belonging to the main classes of alkaloids characteristic for *Lycopodium* spp., e.g. the lycopodane group.

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# PP72. Essential oils from the Herba and fruits of *Peucedanum luxurians* and their antituberculosis activity

*Jarosław Widelski*[1]*, Joanna Golus[2], Rafał Sawicki[2], Grażyna Ginalska[2], Tomasz Mroczek[1], Krystyna Skalicka-Woźniak[1]

*Keywords*: *Peucedanum luxurians*, *Mycobacterium tuberculosis*, H37Ra

The Apiaceae family has been accompanying people for thousands of years, being present in the kitchen, as well as in the pharmacy. Plants belonging to this family are well known as sources of coumarins and essential oils.

Essential oils from the Herba, as well as fruits, of *Peucedanum luxurians* Tamamsch. (an endemic umbelliferous plant taxon from Armenia) were obtained by hydrodistillation in a Deryng apparatus for the first time. The GC-MS analyses showed the presence of *trans*-β-farnesene (16%) and germacrene D (13%) as the most abundant components of the essential oils.

One of the most valuable properties of essential oils is their antimicrobial activity. It is a very desirable feature, especially in the case of some bacteria, which cause huge health problems. A good example is *Mycobacterium tuberculosis*, one of the leading causes of human morbidity and mortality.

The activity of essential oils from different parts of *P. luxurians* was tested for antituberculosis activity. Minimal Inhibitory Concentrations (MIC) values for the essential oils were determined by a 96-well microplate method with alamarBlue (Invitrogen). The inoculum of the reference strain of *Mycobacterium tuberculosis* H37Ra in Middlebrook 7H9 broth (Difco) was 5 x $10^5$ cfu/mL per well, according to CLSI standards. Serial twofold dilutions of essential oils ranged from 8 to 256 µg/mL. As the internal control of the method, serial twofold dilutions of four first-line antibiotics dedicated to tuberculosis treatment: isoniazid (INH), rifampicin (RMP), ethambutol (EMB), and streptomycin (SM) were used [1,2].

*References*:

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[2] Wayne, P.A., 2011. Susceptibility Testing of Mycobacteria, Nocardiae, and Other Aerobic Actinomycetes; Approved Standard-Second Edition. CLSI document M24-A2, Clinical and Laboratory Standards Institute, USA.

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## PP73. Volatile constituents of several *Seseli* species with acetylcholinesterase activity

*Jarosław Widelski*[1]*, Alev Onder[2], Ahsen Sevde Cinar[2], Tomasz Mroczek[1], Krystyna Skalicka-Woźniak[1]

*Keywords*: acetylcholinesterase activity, *Seseli*, GC-MS

Apiaceae is a well-known family of plants with characteristic umbels comprising a lot of aromatic plants important from the economic, medical and ecological points of view. Species from the *Seseli* L. genus are used in traditional medicine since ancient times from their antimicrobial, antiinflammatory and analgesic activities. Plants belonging to the genus *Seseli* are also a rich source of coumarin compounds of different type, which show the ability to inhibit several important enzymes, e.g. acetylcholinesterase (inhibitors of AChE are used in Alzheimer's disease treatment).

Extracts containing volatile compounds were prepared from several *Seseli* representatives (*S. elatum* subsp. *osseum* (Crantz) P.W.Ball, *S. andronakii* Woronow ex Schischk., *S. hartvigii* Parolly & Nordt, and *S. petraeum* M. Bieb.). AChE-inhibitory activity of the tested extracts from *Seseli* species was determined by TLC-bioautography on TLC plates (0.2-mm thickness) covered with silica gel. All TLC plates were developed with the optimized the mobile phase system containing an optimal concentration of 2-naphthyl acetate (30 mg/20 mL).

The GC-MS analysis was carried out on a Shimadzu GC-2010 Plus chromatograph coupled to a QP2010 Ultra mass spectrometric detector using a Phenomenex capillary column ZB-5MS (30 m; diameter of 0.25 mm and thickness of 0.25 µm). The initial column temperature was set to 50 °C, which was held for 3 min, and in the next step, the column was heated to 250 °C at a rate of 8 °C per min (and was then held at that temperature for 2 min). The split ratio after the injection of 1 µL was 1:20 and helium was used as the carrier gas (the flow rate was 1 mL per min). Ionization was performed by electron impact at 70 eV. The identification of compounds was based on a comparison of their mass spectra with those of MassFinder and NIST mass spectral libraries, as well as by retention index (calculated based on a homologous series of *n*-alkanes) comparison.

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# PP74. The essential-oil content and components of *Thymus syriacus* Boiss. at different harvesting periods

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*Keywords*: *Thymus*, carvacrol, essential oil, GC-MS

The genus *Thymus* (Lamiaceae) has 39 species and 59 taxa in the flora of Turkey and 53% of them are endemic. *Thymus syriacus* Boiss. is known to give positive results against cough and other respiratory complaints, as well as some gastrointestinal disorders. Despite the presence of such evidence, scientific investigations concerning the therapeutic use of *T. syriacus* or the aspects of its chemical inventory remain inadequate. In this study, *T. syriacus* leaves were collected from the wild-growing flora of Hatay province at two different phenological periods (pre-flowering and full flowering). The essential oils were obtained from the leaves of *T. syriacus* by hydrodistillation. The essential oil content amounted to 2.25% in the pre-flowering period, while during the full flowering period, the essential-oil content was found to be 2.35%. The essential oils were analyzed by GC/MS. In total, 42 components representing 99.5% of the detected GC-peak areas were identified in the pre-flowering period oil, and 47 representing 98.8% of the detected components of the essential oil hydrodistilled from plant samples collected at the full flowering stage. Carvacrol (82.0-85.7%) was the main component of the essential oils in both pre-flowering and full flowering periods. It was followed by thymol (3.1-4.0%), *o*-cymene (3.1%), γ-terpinene (1.0-2.3%), and β-caryophyllene (0.9-1.3%). In our study, the relative amount of carvacrol was higher compared to the previous studies. There were no significant differences in the relative amount of carvacrol between the harvesting periods. Our study suggests that *T. syriacus*, collected at both phenological phases, could be considered a rich source of carvacrol.

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# PP75. Effects of acorenone-type *Acorus calamus* essential oil on rat gastric fundus contractions and intestinal transit

*Milan Nešić*[1]*, Nikola Stojanović[2], Pavle Ranđelović[2], Niko Radulović[1]

*Keywords*: *Acorus calamus*, essential oil, gastric ulcer, rats

In Serbia and the surrounding countries, *Acorus calamus* L. (Acoraceae) rhizome decoction is frequently used for the treatment of different gastrointestinal disorders, especially gastric ulcers [1]. The rhizomes are rich in the essential oil, to which the rhizomes' bulk activity is assumed to be attributed to. Nowadays, a large number of patients is affected by gastrointestinal disorders and the discovery of new treatments, especially those with an ethnomedicinal history, involving natural volatiles, is very welcome. In the work, we aimed to evaluate the effects of *A. calamus* essential oil on isolated rat fundus contractile abilities and intestinal transit following charcoal application. Commercial *A. calamus* rhizomes produced upon hydrodistillation a high yield of the essential oil (1.08%, w/w). The composition of the oil was analyzed by GC and GC/MS and about one hundred constituents, accounting for 89.3% of the detected GC peak areas, were successfully identified. Acorenone (16.1%), β-asarone (5.8%), camphor (5.6%), and camphene (5.5%) were the most abundant components with recognized biological activities, followed by isoshyobunone (4.2%) and shyobunone (3.0%). The gastric fundus muscle was isolated from healthy female Wistar rats and mounted in a vertical bath, containing Krebs solution, for isolated organs to which increasing concentrations of the essential oil were added (0.01-100 μg/mL). For the intestinal transit experiment, rats were divided into 5 experimental groups (6 rats/group) and were deprived of food 24 h before the experiment. The essential oil (50, 100 and 200 mg/kg) or atropine (2 mg/kg) were orally applied to animals 1 h before a charcoal suspension was given by gavage, while the animals from the control group remained untreated. Thirty minutes later, the animals were sacrificed and the lengths of the small intestine and the path traveled by charcoal were measured. The obtained results revealed that the essential oil, at a concentration of 10 and 100 μg/mL, significantly inhibited the spontaneous fundus contractions. Atropine and all tested doses of the essential oil produced a significant inhibition of the intestinal transit by reducing the length of the path traveled by charcoal. The present results indicate that the essential oil of *A. calamus* significantly affects rat gastrointestinal motor activity by reducing the gastric fundus spontaneous contractions and charcoal intestinal transit.

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## PP76. Biological activity evaluation of Carvi aetheroleum and its major components

*Gözde Öztürk*[1]*, Fatih Demirci[1], Betül Demirci[1]

*Keywords*: *Carum carvi* L., essential oil, antimicrobial activity, *Caenorhabditis elegans*, toxicity

Caraway, *Carum carvi* L. (Apiaceae), is a biennial or annual herb common in Europe, West Asia, and Africa [1]. *C. carvi* essential oil – Carvi aetheroleum is commonly used for flavor, fragrances, and pharmaceutical preparations. In traditional medicine, the essential oil is used as an antispasmodic, for the spastic gastrointestinal tract, diuretic, antimicrobial, and antioxidant, among other uses [2].

In the present study, Pharmacopoeia grade essential oil from commercial sources was evaluated for its antibacterial properties and *in vivo* toxicity. The chemical composition of *C. carvi* essential oil, analyzed by GC/FID and GC/MS, simultaneously, revealed carvone (61.1%) and limonene (37%) as the major constituents. The potential *in vitro* antimicrobial activities of the essential oil and the major components carvone, (+)-limonene and (-)-limonene were evaluated using the broth microdilution assay [3]. *Escherichia coli* NRRL B-3008, *Bacillus cereus* NRRL B3711, *Salmonella typhimurium* ATCC 13311 and *Streptococcus sanguinis* ATCC 10556 were used as the test microorganisms. Based on the determined values of Minimum Inhibitory Concentrations (MIC) for the essential oil and the major constituents, the activities were relatively low (>1000 mg/mL). Lethal concentrations (acute toxicity) were determined by the *in vivo Caenorhabditis elegans* test [4] and the value of $LC_{50}$ <25 mg/mL was obtained.

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# PP77. The activity of laurel essential oil (crude and fractions) in the control of adult bovine ticks and larvae‡

*Carla M. M. Fernandez*[1]*, Maurício F. Rosa[1], Ana Claudia A. M. Fernandez[1], Wanessa C. Bortolucci[2], Giani A. Colauto[2], Nelson B. Colauto[2], Márcia R. Simões[1], Fabiana B. P. Ferreira[3], Viviane S. Lobo[4], Zilda C. Gazim[2]

*Keywords*: *Laurus nobilis*, α-terpineol, linalool, sabinene, *Rhipicephalus (Boophilus) microplus*

Ectoparasites cause direct and indirect losses to farmers, affecting the production of meat and milk and increasing the production costs due to the acquisition of acaricides to maintain cattle health. The financial losses caused by *Rhipicephalus* (*Boophilus*) *microplus*, which is the main livestock ectoparasite in Brazil, reach approximately US$ 3 billion annually. The aim of this study was to evaluate the acaricidal effect of the crude essential oil (EO) and EO's fractions (FR) obtained from *Laurus nobilis* L. (Lauraceae) leaves on *Rhipicephalus* (*Boophilus*) *microplus*. Eight fractions were obtained, wherein five major compounds were identified (sabinene, α-terpinyl acetate, 1,8-cineole, linalool, and α-terpineol). The acaricidal activity of these FR was tested by the larval packet test. The EO was tested by the adult immersion test, and, at concentrations of 200, 100 and 50 µL/mL, the oil caused mortality of engorged females, egg mass reduction, and hatching inhibition. The fractions with α-terpineol and sabinene, as the major compounds, were the most active larvicides ($LC_{50}$=0.13 µL/mL, $LC_{99}$=0.51 µL/mL; and $LC_{50}$=0.20 µL/mL, $LC_{99}$=0.56 µL/mL, respectively). This assessment also indicated that fractionation was important since most of the fractions obtained were more active than the EO. Furthermore, this is the first report of laurel EO and its fractions employed in the control of cattle ticks. Thereby, new prospects for the use of this essential oil or its chromatographic fractions in products applied for cattle tick control can be opened up. However, studies in other stages of development of cattle ticks for the active fractions, and studies under field conditions, the effect on non-target organisms and residual effect on the environment are still needed to evaluate the acaricidal activity of EO and its active fractions.

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# PP78. Antimicrobial activity and *in vivo* toxicity evaluation of *Foeniculum vulgare* Mill. essential oil

*Betül Demirci*[1]*, Gözde Öztürk[1], Fatih Demirci[1]

*Keywords*: *Foeniculum vulgare* Mill., essential oil, antimicrobial activity, *Caenorhabditis elegans*, toxicity

*Foeniculum vulgare* Mill. (Apiaceae) is commonly known as "fennel", a small genus of annual, biennial or perennial herbs distributed in central Europe and the Mediterranean region. It is widely cultivated throughout the temperate and tropical regions of the world for its aromatic fruits, which are used mainly as a culinary spice [1]. Fruits and essential oil of *F. vulgare* are used as flavoring agents in food products, in cosmetic and pharmaceutical products. The essential oil is accredited with antioxidant, antimicrobial, antithrombotic, antidiabetic activities, among others [2].

In this present work, it was aimed to determine the antimicrobial activity of the pharma grade *F. vulgare* essential oil. *trans*-Anethole (68.2%), fenchone (12.8%) and limonene (6.5%) were confirmed as the main constituents; the analysis was performed by GC/FID and GC/MS, simultaneously. Antimicrobial activity of the essential oil was tested against *Escherichia coli* NRRL B-3008, *Bacillus cereus* NRRL B3711, *Salmonella typhimurium* ATCC 13311 and *Streptococcus sanguinis* ATCC 10556 by a broth microdilution assay [3]. Minimum Inhibitory Concentrations (MIC) were found to be: 6.25, 6.25, 3.12 and 12.5 mg/mL, respectively, suggesting that the antimicrobial activity of the essential oil was relatively low against the tested pathogens. In addition, lethal concentration (acute toxicity) was determined using the *in vivo* animal alternative *Caenorhabditis elegans* test [4]. Lethal concentration ($LC_{50}$, 50% of killed nematodes) for the essential oil was determined to be <25 mg/mL.

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## PP79. *In vitro* antimicrobial and anti-mycobacterial activity of *Piper nigrum* Linn. essential oil

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*Keywords*: *Piper nigrum*, essential oil, antimycobacterial, toxicity

In the present study, it was aimed to determine the phytochemical components and evaluate the antimicrobial and antimycobacterial activity of *Piper nigrum* L. (Piperaceae) essential oil. It is well known that black pepper preparations have a wide spectrum of biological activity along with its antimicrobial activity. The antimicrobial properties of black pepper extracts were evaluated previously [1,2].

Commercially available black pepper dried fruits were used as study material. The dry black pepper fruits were pounded, and the essential oil was obtained by hydrodistillation using the Clevenger apparatus. The phytochemical analysis of the essential oil was performed by GC-FID and GC/MS, simultaneously. In addition, *in vitro* antibacterial and antimycobacterial effects against *Staphylococcus aureus*, *S. epidermidis*, methicillin-resistant *S. aureus*, *Streptococcus pyogenes*, *Moraxella catarrhalis*, *Haemophilus influenza*, *Mycobacterium smegmatis*, *M. avium* and *M. fortuitum* subsp. *fortuitum* were assessed by microdilution methods according to CLSI standards [3,4].

The black pepper essential oil was obtained in 10.7 mL/kg yield. According to the GC/FID and GC/MS results, the major constituent of the oil was determined as caryophyllene oxide (28.7%). The antibacterial activity results showed that the oil was effective at different concentrations in the concentration range of 0.16-2.5 mg/mL. According to the antimycobacterial activity results, the essential oil's minimum inhibitory concentrations were 0.08-0.31 mg/mL. LOX-antiinflammatory activity and *Caenorhabditis elegans* toxicity evaluations are under progress for the mode of action and selectivity of the activity.

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# PP80. Biological activity and chemical composition of essential oils from the leaves of *Myrtus communis* L.

*Damla Kırcı*[1]*, Gözde Öztürk[1], Mustafa Eser[2], İbrahim Çavuş[3], Betül Demirci[1]

*Keywords*: *Myrtus communis*, essential oil, antileishmanial, antimicrobial, toxicity

Common myrtle (*Myrtus communis* L., Myrtaceae) is an evergreen shrub. The genus *Myrtus* includes flowering plants and was previously thought to be represented by approximately 16 taxa in the areas of the Middle East and Asia [1]. It has been used for medicinal, food and spice purposes since ancient times. The essential oil is used as an antiseptic, disinfectant, analgesic, and antiinflammatory agent [2,3].

In the present work, *M. communis* leaf essential oil was obtained by hydrodistillation using a Clevenger apparatus. The essential oil was analyzed by both GC-FID and GC-MS. $\alpha$-Pinene (43.1%) and linalool (18.8%) were found to be the main constituents. The oil was evaluated for its toxicity (*Caenorhabditis elegans*), antileishmanial and antimicrobial activities. The $IC_{50}$ value was 2.5 mg/mL against *Leishmania tropica* promastigotes. The following MIC values were determined: *Staphylococcus aureus* ATCC 6538 : 20 mg/mL; *Streptococcus pyogenes* ATCC 13615 : 5 mg/mL; *Candida albicans* ATCC 90028 : 10 mg/mL; and *Escherichia coli* NRRL B-3008 : 1.25 mg/mL. To the best of our knowledge, this is the first report on the *in vivo* selectivity of *M. communis* leaf essential oil against *Leishmania tropica*.

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# PP81. Chemical composition and antimicrobial activity of *Glebionis coronaria* (L.) Cass. ex Spach essential oil

*Esra Yıldırım*[1]*, Hüseyin Servi[2], Betül Eren Keskin[3], Kaan Yılancıoğlu[4]

*Keywords*: *Chrysanthemum coronarium*, essential oils, antimicrobial activity

*Glebionis coronaria* (L.) Cass. ex Spach (syn. *Chrysanthemum coronarium* L.) is a member of the Asteraceae plant family which has extensive edible, folk medicinal, insecticidal uses. Previously, an essential oil of flowerheads of *C. coronarium* from Spain was reported to contain camphor (29.2%), α-pinene (14.8%), β-pinene (9.5%), and lyratyl acetate (9.8%). The oil was shown to possess significant antifungal activity [1]. Also, the essential-oil composition and antimicrobial properties of *C. coronarium* from Ukraine were investigated. The major constituents were found to be chrysanthemyl acetate (24.4%), chrysanthemol (21.8%), chrysanthenyl acetate (7.6%), camphor (7.3%), β-farnesene (5.9%), and α-bisabolol (5.6%). An ethanolic extract of the plant showed antimicrobial activity against Gram-positive (*S. aureus*) bacteria. [2]. Biological activities of the essential oil of *C. coronarium* from Jordan were also reported. The essential oil showed a significant antimicrobial activity against Gram-positive bacteria. Also, the oil showed moderate antioxidant activity, weak acetylcholinesterase-inhibitory and potent antiproliferative activities [3]. In the current study, the essential oil of the aerial parts of *G. coronaria* was obtained by hydrodistillation (3 h). The essential-oil composition was analyzed by means of gas chromatography-mass spectrometry (GC-MS). The main components of the essential oil from the aerial parts were capillene (54.5%) and caryophyllene oxide (9.8%). The current composition differed from the previously reported ones. Thus, *G. coronaria* originating from Istanbul belongs to a new chemotype of this species. Additionally, the antimicrobial activity of the oil was investigated against Gram-negative (*Escherichia coli* DH5α) and Gram-positive (*Staphylococcus aureus*) bacteria. The essential oil showed a growth-inhibitory activity against *E. coli* (53.3%) and *S. aureus* (17.1%), tested at 75 mg/mL. The antimicrobial effects of the essential oil were more pronounced against Gram-negative bacteria.

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# PP82. Chemical composition and antimicrobial activity of *Foeniculum vulgare* Mill. essential oil

*Esra Yıldırım*[1]*, Kaan Yılancıoğlu[2], Betül Eren Keskin[3], Hüseyin Servi[4]

*Keywords*: *Foeniculum vulgare*, essential oils, antimicrobial activity

*Foeniculum vulgare* Mill. (fennel) is a member of the Apiaceae plant family and is used as an antiinflammatory, analgesic, carminative, diuretic, and antispasmodic agent. Nowadays, there is a growing interest in the antioxidant potential and antimicrobial activities of fennel fruit extracts and essential oil [1]. There are many reports on the essential-oil composition of *F. vulgare*. Previously, the composition and significant antimicrobial activity of the essential oil of *F. vulgare* from Pakistan was reported with *trans*-anethole (70.1%) as the main compound [2]. An essential oil of the fruits of *F. vulgare*, containing *trans*-anethole (68.5%) and estragole (10.4%), showed antibacterial activity against *Staphylococcus albus*, *Bacillus subtilis*, *Salmonella typhimurium*, *Shigella dysenteriae*, and *Escherichia coli* [3]. In the current study, the essential oil of the aerial parts of *F. vulgare* was obtained by hydrodistillation (3 h). The essential-oil composition was analyzed by means of gas chromatography-mass spectrometry (GC-MS). The main components of the essential oil from the aerial parts were estragole (33.6%), limonene (24.7%), and α-pinene (19.1%). Additionally, the antimicrobial activity of the essential oil was investigated against Gram-negative (*Escherichia coli* DH5α) and Gram-positive (*Staphylococcus aureus*) bacteria. The essential oil showed a growth inhibitory activity against *E. coli* DH5α (69.3%), tested at 80 mg/mL. However, no activity of the oil was detected in the case of Gram-positive bacteria.

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# PP83. Essential oils of *Calamintha nepeta*, *Origanum vulgare* and *Thymus mastichina* from Alentejo (Portugal): a pharmacological approach

*Sílvia Macedo Arantes*[1,2]*, Andreia Piçarra[1], Marisa Guerreiro[1], Cátia Salvador[1], Fátima Candeias[2,3], A. Teresa Caldeira[1,3], M. Rosário Martins[1,2,3]

*Keywords*: essential oils, *Calamintha nepeta* (L.) Savi subsp. *nepeta*, *Origanum vulgare* L., *Thymus mastichina* L. subsp. *mastichina*, biological properties

Alentejo, in the south of Portugal, is rich in endemic aromatic plants, that are used as condiments and food additives by the local population. Aromatic plants and their essential oils (EOs) have an important role in the protection against oxidative stress, often associated with some diseases, such as atherosclerosis, neurodegenerative and autoimmune diseases, and cancer [1]. The aim of this study was to evaluate the antioxidant, antimicrobial and antiproliferative activities of EOs of autochthones *Calamintha nepeta* (L.) Savi (syn. *Clinopodium nepeta* (L.) Kuntze), *Origanum vulgare* L., and *Thymus mastichina* L. EOs were extracted from the aerial part of the plants by hydrodistillation and the chemical composition was analyzed by GC-FID and GC-MS [2]. Antioxidant potential of the oils was evaluated by three different assays: DPPH radical, β-carotene/linoleic acid and reducing power methods [2]. Antimicrobial activity of the oils was evaluated by a solid disk diffusion assay and minimal inhibitory concentrations (MIC) were determined by a microdilution broth method [2]. Toxicity of the EOs was screened by the brine shrimp lethality test ($LC_{50}$) and the oral lethal doses ($DL_{50}$) were determined for mice [2]. Cell viability was assessed by the MTT (3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide) assay using MDA-MB231 breast cancer cells [3]. EOs were rich in oxygenated monoterpenes and *O. vulgare* EO contained the highest amount of monoterpene hydrocarbons, which have a significant antioxidant potential, i.e. a high ability to protect lipid substrates. EOs were shown to be highly toxic to *A. salina* but of low toxicity to mice. The antibacterial activities were observed against Gram-positive and Gram-negative bacteria. The oils also exhibited a high antiproliferative potential. In conclusion, the antioxidant, antimicrobial and antiproliferative properties of the essential oils of these flavouring herbs point out to their potential use as food supplements and/or in pharmaceutical formulations.

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# PP84. Chemical composition of the essential oil of *Ziziphora clinopodioides* Lam. (Lamiaceae) from Georgia

*Milica Todorovska*[1*], Niko Radulović[1*], Vladimir Ranđelović[2]

*Keywords*: *Ziziphora clinopodioides*, essential oil, pulegone, Georgia

Taxa belonging to the *Ziziphora* L. genus are represented in the Caucasian flora [1,2] and are commonly used in traditional food and for medicinal purposes [2]. *Ziziphora clinopodioides* Lam. (Lamiaceae), known as blue mint bush is widespread in the Caucasus region and used to treat gastrointestinal disorders and as an aperitive, carminative, antiseptic and wound healing material [2]. To the best of our knowledge, there are limited data on the composition of *Z. clinopodioides* essential oil and no previous studies of the essential-oil constituents of *Z. clinopodioides* aerial parts from Georgia. The plant material used for the present study was collected near Jvari Monastery, Mtskheta, Georgia and subjected to hydrodistillation for 3 h using a Clevenger-type apparatus to produce the essential oil. The essential oil was analyzed by GC and GC-MS and this allowed the identification of 28 constituents representing 99% of the total detected GC-peak areas. The essential oil of *Z. clinopodioides* aerial parts from Georgia was found to be characterized by high levels of oxygenated monoterpenes, with the main components identified as pulegone (29.4%), *p*-menth-3-en-8-ol (15.2%), germacrene D (9.2%), neomenthol (5.6%), *cis*-pulegol (5.3%), menthofuran (4.5%), piperitenone (4.3%) and piperitone (3.1%). Pulegone, the most abundant constituent, is a widespread component of the Lamiaceae essential oils [3], however, it has been proven to be highly toxic to laboratory animals, primarily expressing pulmonary and hepatotoxic effects [4]. Having in mind that pulegone represents almost one-third of the oil, further toxicological studies of the *Z. clinopodioides* aerial parts essential oil are needed.

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## PP85. Composition of the essential oil of fennel (*Foeniculum vulgare* Mill.) fruits from Serbia

*Milica Todorovska*[1]*, Niko Radulović[1], Danijela Kostić[1]

*Keywords*: *Foeniculum vulgare*, fennel, essential oil, Serbia

Fennel (*Foeniculum vulgare* Mill.) is a renowned aromatic plant species belonging to the Apiaceae family. Apart from being an ingredient of pharmaceutical and cosmetics products, fennel fruit essential oil is used to flavor liqueurs, bread, pickles and pastries [1]. Many phytochemical studies have been conducted so far to investigate the chemical composition of the essential oil of fennel of different origin, but only few from Serbia [1,2]. The present paper focuses on the chemical composition of the essential oil of fennel fruits (schizocarps) from Serbia. The essential oil, obtained by hydrodistillation carried out using the original Clevenger apparatus, was characterized by gas chromatography (GC) and gas chromatography/mass spectrometry (GC–MS). The oil was obtained in a yield of 1.61% (w/w). In total, 14 components were identified, accounting for more than 98% of the detected total peak areas. *trans*-Anethole (91.4%), a phenylpropanoid, was found to be the main component. Limonene (5.1%) was the second most abundant compound detected, followed by fenchone (2.2%), while all others were found to be the minor contributors. The chemical profile from the present study was similar to the previously reported results [1,2]. In our investigation, the concentration of *trans*-anethole was similar to that in the Coşge and co-workers' study, while the essential oil contained significantly more limonene and fenchone compared to the same work [3]. This could be the effect of genetic structures and ecological conditions affecting the plant. Agricultural practices also have critical effects on the yield and oil composition in essential-oil crops, significantly varying the percentage of main components [4].

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# PP86. Differences in the volatile profile of *Artemisia scoparia* Waldst. & Kit. after a prolonged storage period

*Jovana Ickovski*[1]*, Katarina Stepić[1], Ivan Palić[1], Gordana Stojanović[1]

*Keywords*: *Artemisia scoparia*, essential oil, storage, capillene, capillin

The chemical composition of the essential oils obtained by hydrodistillation of the aerial parts of *Artemisia scoparia* Waldst. & Kit. (Asteraceae) from Serbia immediately after drying (EOI) and after a storage period of one year (EOS) were analyzed by gas chromatography and gas chromatography-mass spectrometry. The comparison of the obtained data for EOI and EOS revealed: a decrease in the oil yield from 0.126% to 0.088%, an increase in the number of components from 22 (representing 99.8% of the total detected GC-peak areas) to 65 (representing 98.6% of all GC-peak areas), and a significant variation in the content of the main constituents. The major component of both oils was capillene (EOI: 57.2%, EOS: 35.2%). During the prolonged storage period, capillene content was found to decrease, whereas capillin content increased (EOI: 0.15%, EOS: 7.1%), which could be the result of autoxidation of capillene to capillin. The amount of limonene dropped (EOI: 2.9%, EOS: 1.2%), which is probably the factor leading to the increase in *p*-cymene (EOI: 1.3%, EOS: 2.4%) [1], along with that generated from *γ*-terpinene (EOI: 3.2%, EOS: 0.4%) [2].

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## PP87. Chemical composition and antioxidant activity of the essential oil of *Artemisia alba* Turra

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*Keywords*: *Artemisia alba*, essential oil, antioxidant activity, DPPH, ABTS

The essential oil of the fresh plant material of *Artemisia alba* Turra (collected in Dimitrovgrad, Serbia) was hydrodistilled using a Clevenger-type apparatus and the obtained essential oil was analyzed by GC and GC-MS. The yield of the essential oil was 0.057%, w/w (based on the weight of fresh plant material). Two hundred and eleven different constituents were identified in the volatile fraction of *A. alba* amounting to 98.3% of the total oil. The major volatiles detected were germacrene D (27.8%), *trans*-*p*-mentha-2,8-dien-1-ol (13.3%), an isomer of santalone (7.8%) and 1,8-cineole (5.6%). The antioxidant activity was screened using two different tests: 2,2-diphenyl-1-picrylhydrazyl radical scavenging assay (DPPH) [1] and 2,2'-azino-bis(3-ethylbenzothiazoline-6-sulphonic acid) radical cation decolorization assay (ABTS) [2] and the results were quantified as Trolox equivalents (TE) per milligram of the essential oil weight. The antioxidant activity determined by the DPPH assay was 23.3 μg TE/mg of the essential oil, whereas ABTS was 4.5 μg TE/mg of the essential oil. Double bonds existing in the dominant compounds of the essential oil (germacrene D, *trans*-*p*-mentha-2,8-dien-1-ol) could potentially be free radical binders, which can explain the scavenging activity of the essential oil by free radical inhibition.

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# PP88. Misidentification of an essential-oil constituent due to repeated reporting of wrong RI value: 2-methyl-2-nonen-4-one vs. 6-hydroxy-2,6-dimethyl-2,7-octadien-4-one

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*Keywords*: misidentification, retention index, 5-oxolinalool, *Sambucus nigra* L.

In the absence of a reference sample, the majority of essential-oil constituents is identified by GC-MS based on a comparison of their mass spectra (MS) and retention indices (RI) with available/literature ones. Hence, the credibility of literature data is a significant one. Herein we report a case where erroneous data led to an essential-oil constituent misidentification in several different plant species. While analyzing the composition of the essential oil of elderflowers (*Sambucus nigra* L.) we tentatively identified a compound with an MS and an RI (1215 on an HP-5 column) which were in good conformity with those previously reported for 2-methyl-2-nonen-4-one [1]. Up to date, this compound has been reported as an essential-oil constituent, with very similar RI values, at least six times. In order to verify this identification, we performed a crossed aldol condensation reaction between 2-heptanone and acetone, and identified the different addition and condensation products only to conclude that the essential-oil constituent in question cannot be the aforementioned enone as its RI value was notably lower (1143). As aldol-addition products were found to have RI values about 10 units higher than the condensation products, this prompted us to consider the possibility that the unknown compound is a tertiary alcohol. As its MS contained no peak at *m*/*z* 59, while a peak at *m*/*z* 71 was present, we considered several structural possibilities and concluded that the compound is likely to be 6-hydroxy-2,6-dimethyl-2,7-octadien-4-one (5-oxolinalool), where a tertiary alcohol function exists alongside a double bond, which is consistent with the observed fragmentation. This compound was previously reported to be a constituent of elderflower volatiles [2]. The tentative assignment is also supported by the presence of other oxygenated linalool derivatives in the elderflower essential oil. It follows that one should always approach GC-MS literature data with a degree of caution and rely on co-injections or information gathered from chemical reactions for identification wherever possible.

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## PP89. The content of α- and β- thujones in essential oils: the qNMR approach

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*Keywords*: thujone, essential oil, qNMR, *Salvia*, *Thuja*

The two diastereomeric thujones, (−)-α-thujone and (+)-β-thujone, are cyclopropane-containing monoterpene ketones that naturally occur in a number of higher plants. As components of essential oils of several genera, the most noteworthy ones are *Artemisia*, *Thuja*, and *Salvia*, thujones are often used in perfumery and are the legally limited components of the renown alcoholic drink absinthe.

The unspecific titration methods for the determination of total thujone content in various samples prompted the development of GC-MS and GC-FID methods that are today the most common ones for its quantitation. Although very precise, these methods require pure standards which are not easily obtainable. It has been recently reported that the content of thujone in absinthe can be determined using $^1$H NMR spectroscopy [1].

Herein, we wish to report on the development of a new and fast method, that does not require expensive pure standards of thujones, for the determination of both contents of α- and β-thujone in essential oils using $^1$H qNMR spectroscopy. NMR spectra of essential-oil samples recorded in $CDCl_3$ containing pentachloroethane (as an internal standard) were used for quantitation purposes. In contrast to the previously proposed NMR methodology, wherein the relevant signals fall in a usually crowded interval of chemical shift values, our newly developed method makes quantitive use of the well-separated signals at δ 0.1241 ppm (*dd*, *J* = 5.6, 4.0 Hz, 1 H) and/or –0.0389 ppm (*dd*, *J* = 5.8, 4.0 Hz, 1 H). The values of the integrals of these signals, originating from hydrogen atoms of the cyclopropane ring of α- and β- thujones, respectively, in respect to the integral of the signal of the standard, allowed an easy determination not only the total thujone content but also the content of the two separate diastereomers. We successfully applied this methodology for the determination of thujone content in several essential oils samples, containing total thujones in the range of 4-70% (*w*/*w*).

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# PP90. New unsaturated lactones from the essential oil *of Tordylium apulum* L. (Apiaceae)

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*Keywords*: 12-hexadecen-4-olide, 14-octadecen-4-olide, DMDS derivatization

*Tordylium apulum* L. (Apiaceae) is a wild-growing plant species, widely distributed throughout the Mediterranean area and West Asia. Ethnobotanically speaking, *T. apulum* is mainly used in salads or to flavor savory pies or vegetable soups, while in folk medicine, it was applied to prevent hair-loss and treat 'nervous illnesses', as well as to bring on menstruation and as an expectorant. From a nutraceutical aspect, it was found that *T. apulum* has a high content of *β*-carotene and vitamin E [1]. In this study, we wish to report on the occurrence of two new compounds – two unsaturated lactones – in the essential oil of stems and leaves of *T. apulum*, obtained by hydrodistillation. The plant material was collected in May 2017, near Gevgelija, a city in the south-east of the FYR Macedonia. Initial GC and GC-MS analyses of the *T. apulum* essential-oil sample showed that *γ*-hexadecalactone, *α*-humulene and (5*Z*,9*E*)-farnesyl acetone were the major constituents (24.8%, 13.7%, 8.8%, w/w, respectively). Saturated lactones, *γ*-pentadecalactone, and *γ*-hexadecalactone were tentatively identified based on their mass spectra and retention data. In addition to these, two unsaturated *γ*-lactones were detected: 12-hexadecen-4-olide (4.3%, w/w) and 14-octadecen-4-olide (2.7%, w/w). In order to corroborate the position of the double bonds, the essential-oil sample of *T. apulum* was subjected to dimethyl disulfide (DMDS) derivatization. Characteristic mass fragmentation of DMDS adducts confirmed the position of the double bonds. These two monounsaturated lactones were never previously reported. Related unsaturated lactones occur in nature, such as (4*R*,9*Z*)-hexadec-9-en-4-olide ((*R*)-desmolactone) which is a sex pheromone of multiple taxa in the Cerambycidae genus *Desmocerus* [2], and (–)-(*Z*)-9-octadecene-4-olide (micromolide), isolated from the stem bark of *Micromelum hirsutum*, which showed potent *in vitro* antituberculosis activity [3]. This production of the lactones, both saturated and unsaturated in *T. apulum*, could be the role of adapting to the environment.

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# PP91. The chemical composition of the essential oil of *Hypericum hirsutum* L. from Suva planina (SE Serbia)

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*Keywords*: *Hypericum*, *Hypericum hirsutum* L., essential oil

The genus *Hypericum* (family Hypericaceae) includes over 500 species with a nearly worldwide distribution, missing only from tropical lowlands, deserts, and polar regions. *Hypericum hirsutum* L., known as Hairy St. John's wort, is very similar to the main representative of genus *Hypericum* - *Hypericum perforatum* L. (St. John's wort). *Hypericum hirsutum* has the typical St. John's wort flower about half an inch or more across and a pale yellow color; blunt, oval, translucent-dotted leaves about 2.5-5 cm long on a smooth, hairy and generally unbranched stem up to about 30-60 cm tall. This perennial species is widely distributed throughout Europe (except the Mediterranean region), northwestern Africa, China and southwestern Asia [1].

Herein, we analyzed by GC-MS the composition of the hydrodistilled essential oil from the aboveground parts of *H. hirsutum*, leaves and stems, and brown capsules (with seeds) at the fruiting stage, separately. The yield of both essential-oil samples was rather low (0.038%, and 0.055%, for leaves and stems, and capsules, respectively), based on the weight of air-dried plant material collected from Suva planina, a mountain in southeastern Serbia. The GC-MS analysis allowed the identification of 90 components in the essential oil of the leaves and stems, and 45 components from the essential oil of the capsules, representing ca. 90% of the total GC-peak areas detected (for both samples). The main components of the leaf essential oil were: *n*-nonane (16.8%), *n*-undecane (10.1%), (*E*)-β-farnesene (9.3), caryophyllene oxide (5.0%), spathulenol (4.5%), (*E*,*E*)-α-farnesene (4.0%), δ-cadinene (3.5%), (*E*)-caryophyllene (3.2%), germacrene D (3.0%), and (*E*)-β-ocimene (2.1%); and the main components in the essential-oil sample from the capsules were: alloaromadendrene (11.5%), caryophyllene oxide (11.1%), *n*-undecane (7.6%), (*E*)-caryophyllene (6.1%), γ-humulene (5.8%), δ-cadinene (5.6%), α-longipinene (5.4%), α-bisabolol (3.6%), and *n*-nonane (3.3%).

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# PP92. The essential-oil composition of *Inula helenium* L. subsp. *turcoracemosa* Grierson from Turkey

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*Keywords*: essential oil, *Inula helenium*, caryophyllene oxide, eudesma-5,11(13)-dien-8,12-olide, isoalantolactone

*Inula helenium* L. (Asteraceae) lipophilic root extracts were previously reported to contain antiproliferative eudesmane (alantolactone derivatives), germacrane and elemane-type sesquiterpene lactones [1]. Additionally, according to a previous report, the essential oil of *I. helenium* roots contained predominantly alantolactone (52.4%), and isoalantolactone (33.0%), while the oil displayed fungistatic and bacteriostatic properties [2]. In the current study, the essential oil composition of the aerial parts of *I. helenium* subsp. *turcoracemosa* collected in Trabzon was determined. The essential oil was obtained by hydrodistillation (3 h) using a Clevenger apparatus. The essential-oil yield was below 0.01% (*v/w*). The essential oil was trapped in *n*-hexane and dried over anhydrous $Na_2SO_4$. The essential oil was analyzed by GC-MS without further dilution. The essential oil was analyzed with an Agilent 5977 MSD GC-MS system operating in EI mode; injector and MS transfer line temperatures were set at 250 °C. Splitless injection was used in the analysis. Innowax FSC column (60 m x 0.25 mm, 0.25 µm film thickness) and helium as the carrier gas (1 mL/min) were used in GC-MS analyses. The oven temperature program was: 60 °C for 10 min and then raised to 220 °C at a rate of 4 °C/min, afterward the temperature was kept constant at 220 °C for 10 min and then raised to 240 °C at a rate of 1 °C/min. Mass spectra were recorded at 70 eV with the mass range *m/z* 35-425. Relative amounts of the separated compounds were calculated from the integration of the peaks in MS chromatograms. Identification of essential-oil components was carried out by comparison of their retention indices (RI), relative to a series of *n*-alkanes ($C_5$ to $C_{30}$), with the literature values, as well as by mass spectral comparison. Ninety-one compounds were identified representing 82.4% of the detected oil constituents. The main components of the oil were caryophyllene oxide (14.7%), eudesma-5,11(13)-dien-8,12-olide (alantolactone, 6.7%), isoalantalactone (3.8%), and aromadendrene oxide (3.3%). The aerial parts oil of *I. helenium* subsp. *turcoracemosa* also contained high amounts of eudesmane sesquiterpenes in accordance with the previous reports on *I. helenium* root essential oil. Our results indicate that eudesmanolides are also present in the aerial parts essential oil.

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# PP93. Probing the existence of chemotypes of *Helleborus odorus* Waldst. & Kit. ex Willd. by essential oil analysis: a multivariate approach

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*Keywords*: *Helleborus odorus*, essential oil, chemotaxonomy, multivariate statistical analyses

*Helleborus* species (family Ranunculaceae) are evergreen, rhizomatous plants with scientifically demonstrated biological/pharmacological activities [1]. Nonetheless, the essential oils of the genus are general poorly phytochemically and pharmacologically investigated. *Helleborus odorus* Waldst. & Kit. ex Willd. ('fragrant hellebore' or 'kukurek' in Serbian) is a highly toxic plant species growing on hillsides and in forests of the submediterranean region. Up to now, steroid-related compounds (saponins, ecdysteroids, bufadienolides), fatty acids and other lipids, and sugars of *H. odorus* were investigated. However, to the best of our knowledge, there are no previous studies of the essential oil of this species.

Analyses by GC and GC/MS of four essential-oil samples obtained from dry aerial parts and roots of *H. odorus* allowed the identification of 229 components, comprising 88.8-92.2% of the total oil composition. The major identified volatile compounds were 1-pentacosene (0.0-52.8%), tricosane (0.0-15.1%), linoleic acid (0.0-11.8%), *trans*-phytol (0.0-12.4%), hexadecanoic acid (3.7-16.8%), (2*E*,4*E*)-decadienal (tr-13.8%), linalool (0.5-6.0%) and hexanal (0.0-7.4%). In general, there were qualitative and quantitative variations noted in the compositions between the *H. odorus* essential-oil samples from different locations. The most discernable differences included a change in the content of the major constituent (1-pentacosene). These differences motivated us to explore (by multivariate statistical analysis (MVA)) the possible existence of several chemotypes of this species using essential-oil compositional data. Agglomerative hierarchical clustering and principal component analysis of the chemical data on the volatiles of the herein studied and additional 37 oil samples of Ranunculaceae showed a close relationship of *Helleborus* with other Ranunculaceae genera and the existence of only one chemotype of this species in the Serbian flora.

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## PP94. Lily of the valley flower volatiles: the chemical composition of the flower diethyl ether extract

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*Keywords*: lily of the valley, fragrance, flowers, phenylacetaldehyde oxime

*Convallaria majalis* L. (Asparagaceae) commonly known as lily of the valley, is popular for the intense and elegant fragrance of the white, bell-shaped flowers. In perfumery, the complex scent of lily of the valley flowers is called the muguet scent. It has something in common with the scent of jasmine, rose and lilac, however, it cannot be imitated by a single compound [1]. In 1956, the French firm Dior created the typical muguet perfume "Diorissimo" (one of the greatest lily of the valley fragrances of all time). Other perfumes imitating or based on this flower scent include "La Muguet" by Annick Goutal, "Muguet" by Guerlain, "Muguet du Bonheur" by Caron, "Varens essential Muguet Secret" by Ulric de Varens etc. The absolute of lily of the valley flowers is used in aromatherapy to help ease headaches, depression, and melancholy; also it is most often found in soaps, creams, and washing powders. However, all parts of this plant are very poisonous; they contain over 30 different types of cardioactive glycosides.

The purpose of this work was to investigate the volatile constituents of a diethyl ether extract of *C. majalis* flowers from Serbia for the first time. GC and GC-MS analyses demonstrated that along components of the flower wax, the main potentially odor-active constituents of the extract were benzyl alcohol, citronellol, geranyl acetate, 2,3-dihydrofarnesol, (*E*)-cinnamyl alcohol, and (*E*)- and (*Z*)-isomers of phenylacetaldehyde oxime. Such a chemical profile was similar to the previously described in the study of the headspace volatiles of lily of the valley flowers [2]. An oxime of phenylacetaldehyde was reported for the first time as a natural product by Sakurai *et al.* in 1979, occurring in the flower of *Citrus unshiu* and that was characterized as one of the compounds responsible for the flower scent [3].

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## PP95. Volatiles of *Pulicaria vulgaris* Gaertn. (Asteraceae)

*Marko Z. Mladenović*[1], Niko S. Radulović[1]*, Nikola M. Stojanović[2], Pavle J. Ranđelović[3], Polina D. Blagojević[1]

*Keywords*: essential oil, *Pulicaria vulgaris* Gaertn., presilphiperfolane diol

The genus *Pulicaria* (tribe Inuleae of the Compositae family) consists of *ca.* 100 species with a distribution from Europe to North Africa and Asia, particularly around the Mediterranean [1]. A number of compounds from *Pulicaria* species (flavonoids, sesquiterpenoids, and diterpenoids) possess significant bioactivities, and they could be promising candidates for the development of potential drugs [1]. In the continuation of our investigations of the secondary metabolites of plant taxa from the Serbian flora, we have studied the chemical composition of *Pulicaria vulgaris* Gaertn. essential oil. *Pulicaria vulgaris* is a rare plant species, with golden-yellow flowers, growing on sandy, stony places. To the best of our knowledge, there are no previous studies on either the volatile or nonvolatile secondary metabolites of this species. Analyses by GC and GC/MS of an essential-oil sample obtained from air-dried aerial parts allowed the identification of 106 components (most of which were identified by at least two independent means (mass spectrum and retention index matching)). Sesquiterpenes constituted the most abundant compound class, representing 86.4% of the total essential oil. The remaining part of the essential-oil sample was comprised of monoterpenes and fatty acid-related compounds, 5.5 and 2.5%, respectively. The bulk of the oil was comprised of two oxygenated sesquiterpenoids–*epi*-α-cadinol (23.3%) and presilphiperfolane-7,8-diol (46.4%). No plant species other than *P. vulgaris* are characterized by the presence of presilphiperfolane-7,8-diol. This fact may be of chemotaxonomic/biosynthetic significance since presilphiperfolanes belong to rare triquinane-type sesquiterpenes that represent precursors of angular and propellane triquinane sesquiterpenes.

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## PP96. Toxicity of carvacrol and its potential in preventing L-arginine-induced pancreatic damage

*Nikola M. Stojanović*[1]*, Milica Stevanović[2], Pavle Randjelović[1], Vladimir Petrović[1], Dušan Sokolović[1], Katarina Mitić[2], Bojan Mladenović[1], Jelena Lalić[1], Niko S. Radulović[2]

*Keywords*: carvacrol, pancreatic tissue, pancreatitis, pathohistological changes

Carvacrol (5-isopropyl-2-methylphenol) is a monoterpene present in the essential oils of many aromatic plants of the Lamiaceae family, including the genera *Origanum*, *Thymus*, *Thymbra*, and *Satureja*. Carvacrol is reported to have a variety of biological properties and its activity might partially be responsible for the activity of ethnomedicinal plants rich in this monoterpene. Our present work aims to estimate the damaging effect of carvacrol on Wistar rat pancreatic tissue, as well as to evaluate its protective action in preventing pancreas damage induced by L-arginine. The toxic and beneficial (in a low dose of 10 mg/kg) properties of carvacrol were assessed by measuring serum α-amylase and lipase activities and tissue malondialdehyde (MDA) content. Also, the pathohistological appearance of pancreatic tissue was assessed, where the presence of edema, inflammation, necrosis, and hemorrhage was scored. The application of higher doses of carvacrol (100 and 500 mg/kg) produced a significant increase in serum α-amylase activity, followed by inflammatory cell infiltration and patchy interlobular edema. In the L-arginine-induced pancreatitis model, a dose of 10 mg/kg of carvacrol was able to prevent the increase in serum α-amylase and lipase activities, as well as to prevent MDA formation compared to the animals that received L-arginine only. Pathological changes also followed the biochemical picture, where mild edema and inflammatory infiltration, with few necrotic areas, could be seen in the tissues of animals treated with carvacrol prior to L-arginine treatment. On the contrary, the tissues of the animals that received L-arginine only displayed massive leukocyte infiltration with edema and significant necrotic areas. One can speculate that the activity of carvacrol is probably arising from its ability to affect the function of multiple cellular mediators, as well as to prevent oxidative tissue damage by mitigating cell oxidative mechanisms.

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# PP97. The floral scent of *Dianthus cruentus* Griseb. (Caryophyllaceae)

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*Keywords*: *Dianthus cruentus*, volatiles, floral scent

The genus *Dianthus* L. (Caryophyllaceae) comprises over 300 species of herbaceous plants that are spread over a vast area, especially in the Mediterranean region. Species of this genus, represented with 38 taxa in the Serbian flora, have attracted attention due to the very beautiful flower color combinations ranging from white to deep purple [1]. This characteristic pigmentation, among several other morphological traits, distinguishes *Dianthus* from other genera within the family Caryophyllaceae, although the evolutionary progress, diversification and the subdivision of the genus still remain controversial [1].

Although *Dianthus* species, especially the flowers, are utilized ethnopharmacologically, only few secondary metabolites, besides pigments, have been studied in detail [1]. A SciFinder search gives back around 4,000 reports dealing with *Dianthus* species, however, less than forty dealt with the analysis of secondary metabolites of the taxa from this genus. Some of the identified constituents displayed a great biological/pharmacological potential, as well as a huge significance for the pollination biology and taxonomy.

*Dianthus cruentus* Griseb. is a highly valued plant species due to the fragrance and blood-red color of its flowers. Strangely, there are no previous reports on its chemical composition in the literature. In this study, we performed the first GC-MS analysis of the volatile constituents of *D. cruentus* flowers in order to possibly detect and identify its odoriferous components.

Only 24 constituents were identified, many of which were easily recognized as having odorous properties. The floral volatiles were made up mainly of fatty acid-derived compounds and shikimate metabolites. The major identified volatile compounds were heptanal, benzyl alcohol, heptanoic acid, maltol, and phenethyl alcohol. All major constituents are well known for its characteristic scent e.g. maltol (odor of cotton candy and caramel), phenethyl alcohol (pleasant floral odor), heptanal (strong fruity odor) etc. Although, maltol might also be an artifact of the analytical procedure and not a true constituent of *D. cruentus* flowers.

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*Acknowledgments*: This work was supported by the Ministry of Education, Science and Technological Development of Serbia [Project No. 172061].

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## PP98. Comparison of the essential-oil composition of *Salvia sclarea* L. aromatherapy oils from Turkish markets

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*Keywords*: essential oil, *Salvia sclarea*, AChE, aromatherapy oils

*Salvia officinalis* does not find a natural habitat in Turkey, however, it is cultivated mostly for export. On the other hand, *Salvia fruticosa* and *S. clarea* are gathered from wild-growing populations, cultivated, used and sold instead of *S. officinalis* for various purposes in Turkey. Previously, the essential-oil composition of *S. sclarea* from various countries was investigated and samples containing linalyl acetate, linalool, germacrene D, α-terpineol, neryl acetate, geraniol, geranyl acetate, nerol, and sclareol were reported [1,2]. In contrast, the essential oil of *S. fruticosa* was reported to contain α-pinene, β-pinene, 1,8-cineole, β-myrcene, and camphor as the main components [3]. In the current study, one aromatherapy-grade essential-oil sample was acquired from a pharmacy and another from a herb shop. Additionally, *clary sage* (adaçayı – local name) was bought from a herb shop and the plant material was used to obtain an essential-oil sample by hydrodistillation using a Clevenger apparatus in the duration of 3 h. The essential oils were analyzed on the Agilent 5977 MSD GC-MS system. The main components of the oil obtained by hydrodistillation were 1,8-cineole (26.8%), camphor (8.9%), α-pinene (6.4%), β-pinene (6.3%), and β-caryophyllene (5.2%). The aromatherapy oil bought from the herb shop contained 1,8-cineole (32.6%), β-caryophyllene (8.7%), camphor (7.3%), α-pinene (6.5%), and β-pinene (5.8%). The aromatherapy oil and the oil obtained from the plant sample sold as *clary sage* had a composition that is similar to that of *S. fruticosa* essential oil. The aromatherapy oil acquired from a pharmacy shop, which is sold as an imported product, contained linalyl acetate (52.1%) and linalool (20.0%) the presence of which is indicative of *S. sclarea* (clary sage) oil. The essential oils were also investigated for their AChE-inhibitory properties. The best noted inhibitory properties of the aromatherapy oil and the hydrodistilled oil were 99±1% and 99.8±0.4%, respectively; whereas the oil sample from pharmacy shop at the same concentration reached the inhibition of 13±2% ($n$ = 3). The results clearly indicate that the products sold as *S. sclarea* on the Turkish market show a great variation due to the misuse of (adulteration with) *S. fruticosa.* This study clearly reveals that further legislation and control is required on the Turkish herbal market in order to protect and inform consumers.

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## PP99. The chemical composition of chives (*Allium schoenoprasum* L.) essential oil

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*Keywords*: *Allium schoenoprasum* L., essential oil, GC-MS analysis, organosulfur compounds

*Allium schoenoprasum* L. (Alliaceae), commonly called chives, is a small bulbous perennial, wild-growing or cultivated, plant widespread in Europe, Asia, and North America. It is commonly used as a culinary herb to impart mild onion flavor to many foods, including salads, soups, vegetables, and sauces. Also, chives are often cultivated in gardens due to their ornamental, as well as insect-repelling properties. However, there are only scarce literature data on the chemical composition of *A. schoenoprasum* essential oil [1,2].

Herein, we performed thorough GC and GC-MS analysis of the essential oil obtained by hydrodistillation of the above-ground parts of *A. schoenoprasum* collected on the Šar Mountains. The analyses of the essential oil revealed that the main class of constituents was the organosulfur compounds representing around 60% of the analyzed oil. Among them, di- and trisulfides bearing a propyl, and alkyl- or alkenyl groups were the most abundant ones. The major component of the oil was methyl propyl trisulfide (8.3%), followed by (*E*)-1-propenyl propyl disulfide (4.6%), dipropyl trisulfide (4.6%), (*E*)-1-propenyl propyl trisulfide (4.5%), and dipropyl disulfide (3.8%). The qualitative composition of the analyzed oil was in a general agreement with the previously reported data [1,2], although the relative abundance of specific compounds differed. A peculiarity about the analyzed oil was that the oil was rich in hetero-penta-/hexa-/hepta- cyclic compounds (containing one or more sulfur and/or nitrogen atoms). Among these, stereoisomeric 4,6-diethyl-1,2,3,5-tetrathianes were the most abundant ones.

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# PP100. The essential-oil composition of *Telekia speciosa* (Schreb.) Baumg. from Trabzon-Turkey

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*Keywords*: essential oil, *Telekia speciosa*, sabinyl acetate, spathulenol, hexadecanoic acid

Previously, the essential oil from the aerial parts of *Telekia speciosa* (Schreb.) Baumg. (Asteraceae) from Serbia was reported to have a complex composition with (*E*,*Z*)-farnesol, (*E*)-nerolidol, β-caryophyllene, caryophyllene oxide, intermedeol, and alantolactone as the main components [1]. The plant material analyzed in the current study was collected in July 2017 from Maçka-Trabzon with an aim to identify the chemical constituents of *T. speciosa* essential oil from Turkey (for the first time) and compare it with the reported oil from Serbia. The essential oil was obtained from air-dried aerial parts of the plant by hydrodistillation (3 h) using a Clevenger apparatus in a yield of 0.06% (*v/w*). The essential oil was diluted 1:10 (*v/v*) with *n*-hexane and used as such for the GC-MS analysis. The essential oil was analyzed with an Agilent 5977 MSD GC-MS system operating in EI mode; injector and MS transfer line temperatures were set at 250 °C. Splitless injection was used in the analysis. Innowax FSC column (60 m x 0.25 mm, 0.25 µm film thickness) and helium as the carrier gas (1 mL/min) were used in GC-MS analyses. The oven temperature program was: 60 °C for 10 min and then raised to 220 °C at a rate of 4 °C/min, afterwards the temperature was kept constant at 220 °C for 10 min and then raised to 240 °C at a rate of 1 °C/min. Mass spectra were recorded at 70 eV with the mass range *m/z* 35-425. Relative amounts of the separated compounds were calculated from the integration of the peaks in MS chromatograms. Identification of essential-oil components was carried out by comparison of their retention indices (RI), relative to a series of *n*-alkanes ($C_5$ to $C_{30}$), with the literature values, as well as by mass spectral comparison. One hundred thirty-four compounds were identified representing 80.5% of the detected oil constituents. The main components of the oil were caryophyllene oxide (8.2%), β-caryophyllene (6.0%), precocene II (3.9%), isoalantolactone (3.5%), *trans*-phytol (2.9%), nerol (2.9%), hexadecenoic acid (2.6%), neryl propionate (2.5%), and thymohydroquinone dimethyl ether (2.3%). The oil composition of *T. speciosa* was very complex as reported previously [1], but the yield in the present study was higher. Caryophyllene oxide and β-caryophyllene were both detected in *T. speciosa* from Turkey and Serbia. However, the Turkish oil did not contain (*E*,*Z*)-farnesol and (*E*)-nerolidol. The AChE-inhibitory activity of the essential oil was 8±1% at 10 mg/mL.

*Reference*:
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# PP101. Composition and AChE-inhibitory properties of *Mentha longifolia* (L.) Hudson subsp. *typhoides* (Briq.) Harley var. *typhoides* (L.) Hudson essential oil

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*Keywords*: essential oil, *Mentha longifolia*, AChE, dihydrocarvone, isodihydrocarvone

There are many reports on the essential-oil composition of the subspecies of *Mentha longifolia* (Lamiaceae). As an example, the essential oil of the *capensis* subspecies from South Africa was reported to contain menthone (50.9%), pulegone (19.3%), and 1,8-cineole (11.9%) [1]. Another report indicated carvone (67.3%), limonene (13.5%), and 1,8-cineole (5.4%) as the main components of *M. longifolia* subsp. *schimperi* oil [2]. Previously, ten different chemotypes of *M. longifolia* subsp. *typhoides* var. *typhoides* were reported in the Tokat flora [3]. Various chemotypes were also detected from Northern Turkey and from the Marmara region [4,5]. In the current study, the essential-oil composition of *Mentha longifolia* (L.) Hudson subsp. *typhoides* (Briq.) Harley var. *typhoides* (L.) Hudson from Maçka–Trabzon was investigated. The essential oil of the aerial parts of the plant was obtained by hydrodistillation (3 h) using a Clevenger apparatus. The essential-oil yield was found to be 0.65% (*v/w*). The essential oil was dried over anhydrous $Na_2SO_4$. The essential oil was diluted with *n*-hexane (1:10, *v/v*) and analyzed as such by GC-MS. The analysis was performed on an Agilent 5977 MSD GC-MS system. Ninety-one compounds were identified in the essential oil representing 97.2% of the detected oil constituents. The main components of the oil were isodihydrocarvone (31.4%), dihydrocarvone (14.5%), β-caryophyllene (9.2%), and limonene (7.5%). A similar carvone-rich chemotype was reported previously [5]. The essential oil was also demonstrated to cause 33.1±0.9%; 29±3%; 5.4±0.4% ($n$=3) of inhibition of AChE activity, at 10, 5 and 1 mg/mL, respectively.

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## PP102. Composition and AChE-inhibitory properties of *Hypericum calycinum* L. essential oil

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*Keywords*: essential oil, *Hypericum calycinum*, AChE, β-pinene, α-pinene

The genus *Hypericum* (Hypericaceae) is represented by 94 taxa in Turkey. *Hypericum* species are very well known due to their uses in folk medicine. There is a considerable number of studies done on *Hypericum* species available in the literature. Previously, the essential-oil composition of *Hypericum calycinum* L. obtained by microdistillation was reported. According to this report, the main components of the oil were α-pinene (24.2%), β-pinene (14.2%), myrtenal (4.5%), verbenone (4.5%), and *trans*-pinocarveol (4.2%) [1]. In the current study, the essential-oil composition *H. calycinum* collected from Şile–İstanbul was determined. The essential oil was obtained by hydrodistillation from aerial parts of the plant with a Clevenger apparatus for 3 h. The essential oil yield was 0.7% (*v/w*). The oil was dried over anhydrous $Na_2SO_4$. The essential oil was diluted 1:10 (*v/v*) in *n*-hexane and analyzed by GC-MS analysis. The essential oil was analyzed with an Agilent 5977 MSD GC-MS system operating in EI mode; injector and MS transfer line temperatures were set at 250 °C. Splitless injection was used in the analysis. Innowax FSC column (60 m x 0.25 mm, 0.25 µm film thickness) and helium as the carrier gas (1 mL/min) were used in GC-MS analyses. The oven temperature program was: 60 °C for 10 min and then raised to 220 °C at a rate of 4 °C/min, afterwards the temperature was kept constant at 220 °C for 10 min and then raised to 240 °C at a rate of 1 °C/min. Mass spectra were recorded at 70 eV with the mass range *m/z* 35-425. Relative amounts of the separated compounds were calculated from the integration of the peaks in MS chromatograms. Identification of essential-oil components was carried out by comparison of their retention indices (RI), relative to a series of *n*-alkanes ($C_5$ to $C_{30}$), with the literature values, as well as by mass spectral comparison. Fifty-four compounds were identified that represented 98.9% of the detected GC-peak areas. The main components of the oil were β-pinene (40.8%), α-pinene (17.7%), limonene (11.9%), and germacrene D (3.3%). The amounts of α- and β-pinene quantified in the oil obtained from Istanbul were found to be different from the previously reported for *H. calycinum* oil. The essential oil obtained from *H. calycinum* originating from Istanbul was characterized by a very high amount of β-pinene. The essential oil caused an 86±1% (*n*=3) AChE activity inhibition at the concentration of 5 mg/mL.

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# PP103. The composition of essential oil of *Veronica persica* Poir. from Istanbul

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*Keywords*: essential oil, *Veronica persica*, phytol, nonacosane, heptacosane

Previously, phenylethanoid and iridoid glycosides were reported from *Veronica persica* Poir. (Plantaginaceae) [1]. However, to the best of our knowledge, there are no reports on its essential oil or volatiles' composition. The aim of the current study was to determine the essential-oil composition of *Veronica persica* to provide information on the chemistry of volatiles of this species. The plant material used in this study was collected from Kanuni Sultan Süleyman City Forest in Istanbul in January 2015. The essential oil of air-dried aerial parts of *V. persica* was obtained by hydrodistillation (3 h) using a Clevenger-type apparatus. The essential-oil yield obtained from the distillation of 16.5 g of plant material was below 0.01 mL. The essential oil was trapped in *n*-hexane (1 mL) and dried over anhydrous $Na_2SO_4$. The essential oil was analyzed without further dilution by GC-MS. The essential oil was analyzed with an Agilent 5977 MSD GC-MS system operating in EI mode; injector and MS transfer line temperatures were set at 250 °C. Splitless injection was used in the analysis. Innowax FSC column (60 m x 0.25 mm, 0.25 µm film thickness) and helium as the carrier gas (1 mL/min) were used in GC-MS analyses. The oven temperature program was: 60 °C for 10 min and then raised to 220 °C at a rate of 4 °C/min, afterward the temperature was kept constant at 220 °C for 10 min and then raised to 240 °C at a rate of 1 °C/min. Mass spectra were recorded at 70 eV with the mass range *m/z* 35-425. Relative amounts of the separated compounds were calculated from the integration of the peaks in MS chromatograms. Identification of essential-oil components was carried out by comparison of their retention indices (RI), relative to a series of *n*-alkanes ($C_5$ to $C_{30}$), with the literature values, as well as by mass spectral comparison. *Veronica persica* oil was mainly composed of the diterpene *trans*-phytol and *n*-alkanes. Seventeen compounds were identified representing 92.1% of the detected oil constituents. The main components of the oil were *trans*-phytol (24.4%), nonacosane (15.9%), heptacosane (13.1%), and hentriacontane (7.2%). The essential oil did not contain any monoterpenes but contained sesquiterpenes in only minor amounts. We believe the existence of the diterpene *trans*-phytol in high quantity points to the possibility that other monoterpenes and sesquiterpenes might also be present in the plant, but that they might be observed through headspace or SPME sampling.

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# PP104. The essential-oil composition of *Crocus pestalozzae* Boiss. from Istanbul

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*Keywords*: essential oil, *Crocus pestalozzae*, heptacosane, pentacosane, nonacosane

*Crocus* (Iridaceae) species are well-known for their use as spices. In Turkey, the genus *Crocus* is represented with 62 taxa. In the literature, there is no particular report on the chemistry of volatile or non-volatile secondary metabolites of *C. pestalozzae* Boiss. The aim of the current study was to contribute novel information on the chemistry of the volatile secondary metabolites of *C. pestalozzae*. The plant material used in this study was collected from Kanuni Sultan Süleyman City Forest in Istanbul in January 2016. The essential oil of air-dried aerial part of *C. pestalozzae* was obtained by hydrodistillation (3 h) using a Clevenger-type apparatus. The obtained essential-oil yield was below 0.01 mL. The essential oil was trapped in *n*-hexane (1 mL) and dried over anhydrous $Na_2SO_4$. The essential oil was analyzed by GC-MS without further dilution. The essential oil was analyzed with an Agilent 5977 MSD GC-MS system operating in EI mode; injector and MS transfer line temperatures were set at 250 °C. Splitless injection was used in the analysis. Innowax FSC column (60 m x 0.25 mm, 0.25 µm film thickness) and helium as the carrier gas (1 mL/min) were used in GC-MS analyses. The oven temperature program was: 60 °C for 10 min and then raised to 220 °C at a rate of 4 ˚C/min, afterward the temperature was kept constant at 220 °C for 10 min and then raised to 240 °C at a rate of 1 °C/min. Mass spectra were recorded at 70 eV with the mass range *m/z* 35-425. Relative amounts of the separated compounds were calculated from the integration of the peaks in MS chromatograms. Identification of essential-oil components was carried out by comparison of their retention indices (RI), relative to a series of *n*-alkanes ($C_5$ to $C_{30}$), with the literature values, as well as by mass spectral comparison. Fifty-four compounds were identified representing 86.2% of the detected oil constituents. The main components of the oil were heptacosane (18.2%), pentacosane (17.0%), nonacosane (13.1%), heneicosane (7.2%), and 1-docosanol (5.3%). Safranal and its derivatives were detected in the essential oil but only in very small amounts. Due to the low amounts of safranal and other commonly observed volatile compounds of *Crocus* species [1], one would expect to observe a different volatile secondary metabolite profile if headspace or SPME sampling were employed.

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# PP105. Chemical variability, toxicity, and antibacterial activity against opportunistic pathogens of the essential oils from *Origanum vulgare* (*hirtum* x *viridulum*)

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*Keywords: Origanum vulgare*, essential oil, antimicrobial activity, opportunistic pathogens

The genera *Citrobacter*, *Bacillus*, *Shigella*, and *Pseudomonas* include overt and opportunistic pathogens responsible for a wide range of infections that are the causes of sporadic septicemia, pneumonia, and digestive and urinary tract infections. The presence of high amounts of phenolic compounds in essential oils provides an insight into the likely effect of a specific chemotype against opportunistic pathogens. The main goal of the present work was to evaluate the bacterial growth inhibition by five *Origanum vulgare* L. (Lamiaceae) essential oil chemotypes. The most active chemotype was also tested for intestinal toxicity using an experimental animal model. The bacterial growth inhibition curves against *Pseudomonas aeruginosa* CECT 108, *Shigella sonnei* CECT 413, *Bacillus cereus* CECT 131, and *Citrobacter freundii* CECT 7464 were set up. The following parameters were assessed from the animal model experiments: villius height, Lieberkühn crypt depth, and intestinal mucosal thickness. A total of 15 individual plants (3 per chemotype) were used in this assay. The essential oils were extracted by hydrodistillation and the qualitative and quantitative compositions were analyzed using a gas chromatograph coupled to a mass spectrometer (GC-MS). The growth inhibition curves were constructed for the 48-h treatment and the tested essential-oil concentrations ranged from 40 to 1250 ppm for *S. sonnei*, *B. cereus*, and *C. freundii*, and from 625 to 20000 ppm for *P. aeruginosa*. The GC-MS results revealed that the tested chemotypes were composed of: 86% of carvacrol; 77% of carvacrol and 6% of thymol; 65% of carvacrol and 18% of thymol; 48% of carvacrol, 12% of γ-terpinene, and 6% of caryophyllene; 34% of carvacrol, 15% of γ-terpinene, 8% of *p*-cymene, and 7% of caryophyllene.

*From results it can be concluded*: that among the chemotypes studied, the ones having over 48% of carvacrol in the oil inhibited the growth of *S. sonnei* and *B. cereus* (312 ppm), and *C. freundii* (625 ppm). In the case of *P. aeruginosa*, only chemotypes with a high amount of carvacrol (86-76%) at the highest tested concentration (20000 ppm) were active. In addition, the maximal doses tested did not result in intestinal toxicity.

*Acknowledgments:* This work is part of a project (FEDER 14-20-12) O.P. FEDER 2014-2020.

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## PP106. Anti-*Bacillus cereus* activity of three aromatic plants cultivated in the Region of Murcia (Spain)

*Cristina Martínez-Conesa*[1]*, J. A.Sotomayor[1], P. Sánchez-Gómez[2], I. García[1], P. Romero[1], M. Quílez[1], M. J. Jordán[1]

*Keywords*: *Origanum vulgare*, *Salvia lavandulifolia*, *Thymus hyemalis*, essential oil, antimicrobial activity

*Bacillus cereus* is a Gram-positive, endospore-forming, opportunistic human pathogen that causes two types of food-poisoning syndrome: emesis and diarrhea. The trend towards Refrigerated Processed Foods of Extended Durability (REPFEDs) and the increasing percentage of elderly and immunocompromised people will raise the importance of *B. cereus* as an aetiological agent of food-borne illness. *The aim of this work* was to evaluate the chemical variability of the essential oils of three Lamiaceae taxa: *Origanum vulgare* L., *Salvia officinalis* subsp. *lavandulifolia* (Vahl) Gams (syn. *Salvia lavandulifolia* Vahl), and *Thymus hyemalis* Lange in relation to their antibacterial activity against *B. cereus* strain CECT 131. A total of 30 individual plants (10 from each species) were used in the assay. The essential oils were extracted by hydrodistillation and the qualitative and quantitative compositions were analyzed using a gas chromatograph coupled to a mass spectrometric detector (GC-MS). The minimal inhibitory concentrations (MIC) were determined by a microdilution technique, using 96-well microplates. The minimal bactericidal concentrations (MBC) were established by pour-plating. To determine if the vegetative form or the endospore was the cause of the bacterial growth, Würtz staining was used: malachite green binds to the endospores and is used as a contrast dye, while safranin stains the vegetative cells. The tested concentrations of the essential oils ranged from 40 to 10000 ppm for *O. vulgare* and *T. hyemalis*, and from 1875 to 60000 ppm for *S. lavandulifolia*. The herein tested essential-oil chemotypes of *O. vulgare* were: (A) 86% of carvacrol, (B) 77% of carvacrol and 6% of thymol, and (C) 65% of carvacrol and 18% of thymol; the chemotypes of *S. lavandulifolia* were: (D) 37% of camphor, 11% of α-pinene and 8% of eucalyptol, (E) 22% of camphor and 25% of eucalyptol, and (F) 55% of eucalyptol and 13% of camphor; and for *T. hyemalis*, the chemotypes were: (G) 52% of carvacrol and 25% *p*-cymene, (H) 50% of thymol, 25% of *p*-cymene and 10% of γ-terpinene, and (I) 44% of *p*-cymene and 41% of thymol. *From the results it can be concluded*: that the highest antimicrobial power was exhibited by chemotypes A of *O. vulgare* and G of *T. hyemalis* (MIC = 156-312 ppm), for the exposure times of 24 and 48 h. In the case of *S. lavandulifolia*, the lowest MIC was that of chemotype D in the concertation range 5000-60000 ppm. The MBC for the endospores, for all the chemotypes tested, was higher than the concentrations evaluated.

*Acknowledgments:* This work is part of a project (FEDER 14-20-12) O.P. FEDER 2014-2020.

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# PP107. AChE-inhibitory properties and the chemical composition of *Salvia aethiopis* L. essential oil

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*Keywords*: essential oil, *Salvia aethiopis*, AChE, germacrene D, α-copaene

Previously, the hydrodistilled essential oil of the aerial parts of *Salvia aethiopis* L. (Lamiaceae) from Erzurum–Turkey was reported to contain germacrene D (29.0%), α-copaene (19.8%), β-cubebene + β-elemene (9.9%), bicyclogermacrene (9.3%), δ-cadinene (8.7%), and β-caryophyllene (7.3%) [1]. The current study aims to provide information on the essential-oil composition of the aerial parts of *S. aethiopis* from another location in Turkey. The plant material used in this study was collected from Tokat in June 2017. The essential oil was obtained by hydrodistillation (3 h) of air-dried aerial parts using a Clevenger-type apparatus, in a yield of 0.09 mL per 100 g of plant material. The essential oil was diluted with *n*-hexane 1:10 (*v/v*) and used as such for the GC-MS analysis. The essential oil was analyzed with an Agilent 5977 MSD GC-MS system operating in EI mode; injector and MS transfer line temperatures were set at 250 °C. Splitless injection was used in the analysis. Innowax FSC column (60 m x 0.25 mm, 0.25 µm film thickness) and helium as the carrier gas (1 mL/min) were used in GC-MS analyses. The oven temperature program was: 60 °C for 10 min and then raised to 220 °C at a rate of 4 °C/min, afterwards the temperature was kept constant at 220 °C for 10 min and then raised to 240 °C at a rate of 1 °C/min. Mass spectra were recorded at 70 eV with the mass range *m/z* 35-425. Relative amounts of the separated compounds were calculated from the integration of the peaks in MS chromatograms. Identification of essential-oil components was carried out by comparison of their retention indices (RI), relative to a series of *n*-alkanes ($C_5$ to $C_{30}$), with the literature values, as well as by mass spectral comparison. Eighty-one compounds were identified comprising 90.1% of the detected oil constitutes. The main components of the oil of *S. aethiopis* from Tokat were α-copaene (17.8%), germacrene D (12.7%), bicyclogermacrene (11.8%), β-caryophyllene (6.9%), and δ-cadinene (4.3%). The results agreed generally with the literature ones except for the variation in the percentage of the main components. Additionally, AChE-inhibitory properties of the essential oil were investigated and the oil was demonstrated to inhibit 46.4±0.8% ($n$ = 3) of AChE activity, at 1 mg/mL.

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## PP108. A new essential-oil chemotype of *Tanacetum sorbifolium* (Boiss. ex Boiss.) Grierson from Trabzon-Turkey

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*Keywords*: essential oil, *Tanacetum sorbifolium*, sabinyl acetate, spathulenol, hexadecanoic acid

Previously, the essential oil of the aerial parts of *Tanacetum sorbifolium* (Boiss. ex Boiss.) Grierson (Asteraceae) from Gümüşhane-Turkey was reported to contain camphor (54.3%), pinocarvone (5.1%), and bornyl acetate (3.9%) [1]. There are a number of examples of *Tanacetum* species showing a high degree of chemotypification. During our fieldwork in Trabzon, we encountered *T. sorbifolium* and decided to reanalyze its essential oil due to the possibility of finding a new chemotype. The plant material used in this study was collected in July 2017 at an altitude of 1328 m. The essential oil was obtained from air-dried aerial parts by hydrodistillation (3 h) in a Clevenger-type apparatus in a yield of 0.09% (*v/w*). The essential oil was diluted 1:10 (*v/v*) with *n*-hexane and used as such for the GC-MS analysis. The GC-MS analysis was done on an Agilent 5977 MSD GC-MS system operating in EI mode with a split injection (1:50). An Innowax FSC column (60 m x 0.25 mm, 0.25 µm film thickness) and helium, as the carrier gas (1 mL/min), were used. The following temperature program was used in the GC-MS analysis–60 °C: 10 min→ 220 °C at 4 °C/min; 220 °C: 10 min→ 240 °C at 1 °C/min). Identification of essential-oil components was carried out by comparison of their retention indices (RI), relative to a series of *n*-alkanes ($C_5$ to $C_{30}$), with the literature values, as well as by mass spectral comparison. One hundred seventy-four compounds were identified representing 84.1% of the detected GC-peak areas. The main components of the oil were sabinyl acetate (15.4%), spathulenol (7.5%), hexadecanoic acid (2.6%), artemisia ketone (2.4%), caryophyllenol-I (2.4%), salvial-4(14)-en-1ξ-ol (2.3%), and linalool (2.1%). The essential oil composition of *T. sorbifolium* from Trabzon is more complex in comparison to the previously reported composition. Additionally, the main components observed in the current study and those from the literature were considerably different. Previously, camphor, pinocarvone, and bornyl acetate were reported as the main components, however, in the current study, the essential oil completely lacked camphor and pinocarvone but it contained bornyl acetate in only 0.4%. AChE-inhibitory properties of the oil were also investigated and it was found that the oil (at 5 mg/ml) inhibited 7±2% ($n$ = 3) of the enzyme's activity.

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# PP109. The composition of the essential oil of the aerial parts of an endemic new species *Ferula mervynii* Sağıroğlu & H.Duman from Turkey

*Berivan İlhanlı*[1]*, Sibel Barbaros[2], Yasemin Yücel Yücel[3], Bilal Şahin[4], Ömer Cem Karakoç[4], Kaan Polatoğlu[5]

*Keywords*: essential oil, *Ferula mervynii,* α-pinene, β-pinene, sabinene

In 2007, *Ferula mervynii* Sağıroğlu & H.Duman (Apiaceae) was reported as a new species from Turkey. This species finds a natural habitat in Artvin and Erzurum regions that are located in North-Eastern Anatolia [1]. Up to now, there are no reports on the chemistry of this species. However, there are many reports on the essential-oil composition of other *Ferula* species from Turkey. As an example, *F. elaeochytris* Korovin essential oil was reported to have nonane (27.1%), α-pinene (12.7%), and germacrene B (10.3%) as the main components [2], whereas, *F. szowitziana* D.C. was reported to contain β-eudesmol (32.0-29.5%), α-eudesmol (18.2-16.6%), and α-pinene (8.6-6.4%) as the major components of the leaf and stem oils, respectively [3]. The current study aimed to provide information on the chemistry of the essential oil of *F. mervynii* collected from Erzurum, Turkey, in August 2017. The essential oil was obtained by hydrodistillation from air-dried aerial parts of the plant using a Clevenger-type apparatus in the duration of 3 h. The essential-oil yield was determined to be 0.56% (*v/w*). The oil was diluted with *n*-hexane 1:10 (*v/v*) and analyzed as such on an Agilent 5977 MSD GC-MS system. Relative amounts of the separated compounds were calculated from the integration of the peaks in MS chromatograms. Identification of essential-oil components was carried out by comparison of their retention indices (RI), relative to a series of *n*-alkanes ($C_5$ to $C_{30}$), with the literature values, as well as by mass spectral comparison. The aerial parts essential oil of *F. mervynii* was rich in monoterpenes. The major components were α-pinene (48.1%), sabinene (20.0%), β-pinene (11.6%), and terpinen-4-ol (2.5%). The highest AChE-inhibitory activity of the oil was found to reach 51±1% of inhibition of the enzyme activity.

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# PP110. The chemical composition of *Salvia euphratica* Montbret & Aucher ex Benth. essential oil from Sivas-Turkey

*Berivan İlhanlı*[1]*, Sibel Barbaros[2], Yasemin Yücel Yücel[3], Bilal Şahin[4], Ömer Cem Karakoç[4], Kaan Polatoğlu[5]

*Keywords*: essential oil, *Salvia euphratica*, 1,8-cineole, camphor, myrtenal

Previously, only the fatty-oil composition of *Salvia euphratica* Montbret & Aucher ex Benth. (syn. *Salvia euphratica* var. *euphratica*) was reported, however, there are no other studies on the chemistry of this species [1]. Up to now, there are no reports on the essential-oil composition of this taxon. In this study, we aimed to investigate the composition of three different samples of the essential oil of *S. euphratica* collected in June 2017 from two different sites in Sivas-Turkey. The essential oil was obtained by hydrodistillation from air-dried aerial parts of the plant using a Clevenger-type apparatus for the duration of 3 h. The essential-oil yields for the three samples were determined to be: 0.25, 0.15, and 0.13% (*v/v*), for a sample with glandular hairs (1) and a sample without glandular hairs (2) from location 1 and for a sample with glandular hairs (3) from location 2, respectively. The oils were diluted with *n*-hexane 1:10 (*v/v*) and analyzed as such on an Agilent 5977 MSD GC-MS system operating in the EI mode injector and MS transfer line temperatures were set at 250 °C. Splitless injection was used in the analysis. Innowax FSC column (60 m x 0.25 mm, 0.25 µm film thickness) and helium, as the carrier gas (1 mL/min), were used in GC-MS analyses. The oven temperature program was: 60 °C for 10 min and then raised to 220 °C at a rate of 4 °C/min, afterwards the temperature was kept constant at 220 °C for 10 min and then raised to 240 °C at a rate of 1 °C/min. Mass spectra were recorded at 70 eV with the mass range *m/z* 35-425. Relative amounts of the separated compounds were calculated from the integration of the peaks in MS chromatograms. The main components of sample 1 essential oil were 1,8-cineole (20.7%), camphor (10.0%), nopinone (4.7%), *trans*-pinocarveol (4.3%), myrtenal (4.3%), β-pinene (3.3%), and camphene (2.2%). Sample 2 oil contained high amounts of 1,8-cineole (13.5%), camphor (7.6%), *trans*-pinocarveol (7.1%), myrtenal (5.7%), nopinone (4.6%), myrtenol (3.9%), borneol (3.4%), and pinocarvone (3.2%). Finally, the main components of sample 3 oil were: 1,8-cineole (16.8%), *trans*-pinocarveol (4.7%), camphor (4.0%), myrtenyl acetate (3.7%), myrtenal (3.6%), linalool (2.8%), *trans*-linalool oxide (furanoid) (2.6%), and myrtenol (2.6%). The highest noted AChE-inhibitory activity of the oils were 63±5%, 57±2%, and 63±1%, respectively.

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# PP111. Evaluation of the anticancer potential of *Aloysia citriodora* and its major components, isomeric citral, and their potential synergy with conventional chemotherapeutic drugs in human colon carcinoma

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*Keywords*: *Lippia citriodora*, citral, Greece, cell death pathway, chemotherapeutic drugs

*Aloysia citriodora* Palau (syn. *Lippia citriodora* (Palau) Kunth), commonly known as lemon verbena, is a perennial shrub, belonging to the family Verbenaceae, with a very pleasant lemony aroma that was first cultivated in South America and brought to Europe in the 17th century [1]. While its aqueous extracts have been studied a lot for their biological properties, few studies exist on the bioactivities of the essential oil [2]. We previously identified citral (geranial and neral) as the main component of the lemon verbena essential oil (LVO) isolated from Greek plants and showed that they both possess significant antiproliferative activity, with LVO being less genotoxic and more cytoprotective than citrals *in vitro* [3]. The aim of this study was to investigate the mode of antiproliferative action of LVO/citral and their potential synergy effects with conventional chemotherapeutic drugs used in the treatment of colorectal cancer and further study the molecular mechanisms of cytotoxicity of these combinations. Flow cytometry analysis revealed a G2/M arrest of colon cancer cells (Caco2, HT-29) after the treatment with the oil and citral. Neither the oil nor citral induced caspase-dependent cell death, while LVO did not alter significantly the expression of a number of proteins related to apoptosis (Caco2), apart from the proteins survivin, claspin, TRAILR2, clusterin, HSP60, and Fas. Sulforhodamine B assay was conducted after a co-incubation of LVO or citral with irinotecan or oxaliplatin, where both agents showed a synergistic effect with the drugs. Our results further deepen our understanding of the bioactivities of lemon verbena essential oil and citral for their future use as chemopreventive or chemotherapeutic agents in the battle against cancer.

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## PP112. Effect of pH on the synergism of thymol and carvacrol against *Saccharomyces cerevisiae*

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*Keywords*: thymol, carvacrol, synergism, $IC_{50}$, *Saccharomyces cerevisiae*

Thymol and carvacrol are *natural* monoterpene phenols found in high concentration in various essentials oils including the oil of thyme. These monoterpene phenols are known to possess strong antiseptic activities [1]. In this study, I detail the effect that pH has on the synergism of thymol and carvacrol against the model organism, *Saccharomyces cerevisiae*. For every 0.1 unit interval in the pH range (6.4-8.4), $IC_{50}$ values were measured based on the thymol content in the mixture of thymol and carvacrol. The maximum potency of *0.399 mg* $L^{-1}$ was achieved at pH 6.4 using a 1:9 ratio of thymol to carvacrol – over 5 times more potent than thymol alone at pH 7.4 ($IC_{50}$ = 2.05 mg $L^{-1}$). Understanding the synergy of the components in essential oils is one of the first steps in establishing alternative treatments to fight drug-resistant microorganisms. By combining essential oils or their components with existing antibiotic or antifungal agents, effective treatment of *superbugs* can be elucidated [2].

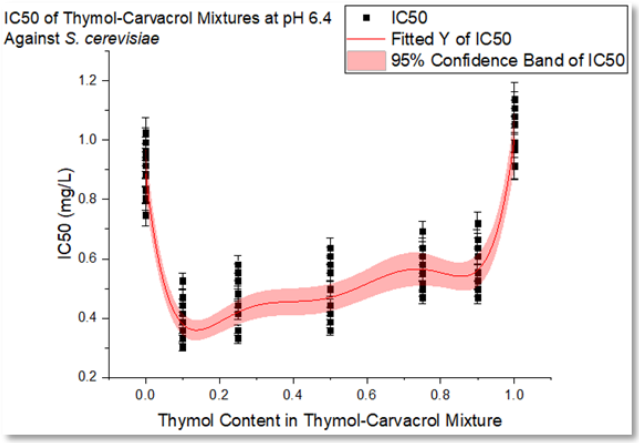


Fig. 1. Graph of all the measured $IC_{50}$ values (mg $L^{-1}$) for the thymol-carvacrol mixture based on the composition of the mixture at pH 6.4 ($R^2$ = 0.880).

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