34th INTERNATIONAL SYMPOSIUM ON ESSENTIAL OILS

Würzburg / Germany
September 7 - 10, 2003

ISEO 2003

Chairmen:
Prof. Dr. K.-H. Kubeczka / Prof. Dr. P. Schreier
University of Würzburg

Program, Book of Abstracts and List of Participants

34th INTERNATIONAL SYMPOSIUM ON ESSENTIAL OILS ISEO 2003

University of Würzburg
September 7 – 10, 2003

PROGRAM

BOOK OF ABSTRACTS

LIST OF PARTICIPANTS

Organization:

Prof. Dr. Karl-Heinz Kubeczka

Prof. Dr. Peter Schreier

The 34th International Symposium on Essential Oils was generously sponsered by:

Adalbert-Raps-Stiftung, Kulmbach

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- IFEAT was founded in 1977. Its aims as determined at that time remain the same today and briefly they can be stated as follows:
- To advance and promote the commercial viewpoint of the essentials oils and aroma chemicals industry world-wide.
- To encourage the production of essential oils and co-operate with international associations representing compounders of essential oils and aromatics.
- To organise international meetings and to develop a constructive dialogue among producers, dealers and users of fragrances and flavour raw materials.
- From those small beginnings, the Federation has developed into a truly international organisation and its members are involved in all aspects of essential oils and aroma chemical production, extraction, brokerage and usage.

IFEAT Website address: www.ifeat.org

General Information

Chairmen of the Symposium: **K.-H. Kubeczka, P. Schreier, Würzburg, Germany**
Honorary Guest: **Prof. Dr. A. Baerheim-Svendsen, Oslo, Norway**

SCIENTIFIC COMMITTEE

Y. Asakawa, Tokushima/Japan
K.H.C. Baser, Eskisehir/Turkey
C. Bicchi, Torino/Italy
G. Buchbauer, Vienna/Austria
A.C. Figueiredo, Lisbon/Portugal
C. Franz, Vienna/Austria
R. Hiltunen, Helsinki/Finland
D. Joulain, Grasse/France
W.A. König, Hamburg/Germany
K.H. Kubeczka, Würzburg/Germany
B. Lawrence, Winston-Salem/USA
R. Naef, Geneva/Switzerland
J.J.C. Scheffer, Leiden/The Netherlands
P. Schreier, Würzburg/Germany
E. Stahl-Biskup, Hamburg/Germany
P. Weyerstahl, Berlin/Germany

LOCAL ORGANIZING COMMITTE

F. Heckel
M. Kraus
Chr. Kubeczka
K.-H. Kubeczka
E. Richling
P. Schreier

Location and time

The conference and poster session will be held in the central building of the Faculty of Chemistry and Pharmacy at the University area „Am Hubland". The symposium will commence on Monday, September 8th at 9.30 and close at 12.45, Wednesday, September 10th.

Registration

The registration desk will be located on September 7th in the restaurant „Residenz-Gaststätten", Residenzplatz 1 in the center of the city; it will be open from 17.00 to 19.00. From Monday to Wednesday it is located in the lounge of the lecture halls in the central building of the Faculty of Chemistry and Pharmacy at the University area „Am Hubland" and will be open on Monday, Sept. 8th from 9.00 and the following days from 8.30 onwards; it closes on Wednesday, Sept. 10th at 12.00.

Oral communications

The plenary lectures are limited to 45 min., oral communications to 20 min., both with additional 5 min. for discussion. Overhead and slide projectors as well as MS-Power Point presentation facilities are available. Slides and CDs should be handed in at the Symposium Office, in the Foyer of the lecture halls, with the corresponding number of the presentation and the name of the presenting author at least 1h prior to the beginning of the respective session.

Posters

The poster boards (120cm wide and 100 height) are located in the passage way around the lecture halls in the central building of the Faculty of Chemistry and Pharmacy „Am Hubland". They are labelled and the number corresponds to the number listed in the program. You are kindly requested to attach your Poster on Monday morning, September 8 and to be present at your poster during the indicated poster session for discussion of your results.
Please take care that the poster should be removed before the end of ISEO 2003 on Wednesday, September 10 around 12.45. Affixing materials will be available at the registration desk.

Lunch

Owing to the short time for lunch, we would highly recommend to take the lunch in the academic canteen "Mensa" (about 50m from the main building) from 12.00 to 14.00.
At the canteen lunch vouchers are requested. They can be purchased at the registration desk (8,-- € per day and meal incl. 1 drink).

Badges

Participants and accompanying persons are kindly requested to wear their Symposium badges for identification and admittance to Scientific and Social venues.

Insurence / Liability

The Organisers are in no respect responsible for any accommodation problem, nor for any accident, injury, loss and property damage to any person during the symposium.

Social Events

Sunday, September 7, 2003

19.00 Get-Together-Party
An informal welcome with a small buffet will be arranged in the 1st floor of the restaurant "Residenz-Gaststätten", Residenzplatz 1, in the center of the city.

Tuesday, September 9, 2003

19.00 Symposium-Dinner
Residence palace, in the center of the city.

Wednesday, September 10, 2003

14.30 Excursion to Weikersheim Castle
There will be the possibility to have snacks and drinks (not included in the fee).
Return in Würzburg at approx. 18.30

34th International Symposium on Essential Oils

September 7 – 10, Würzburg, Germany

Scientific Program

Sunday September 7, 2003

17.00 - 19.00 Registration at the Symposium Office
(Residenz-Gaststätten, Residenzplatz 1)

19.00 - 21.00 Get-Together-Party
(Residenz-Gaststätten, Residenzplatz 1)

Monday September 8, 2003

9.00 Registration at the Symposium Office
(Chemistry central building, Am Hubland)

9.30 **Opening Session**
Welcome Addresses

10.10 Plenary Lecture 1 Chair: Dr. B. M. Lawrence

PL-1 **W.A. König**, Hamburg, Germany
Strategies for the identification of known and unknown essential oil constituents

11.00 Coffee break

11.20 L-01 **L. Mondello** and G. Dugo, Messina, Italy
Ultra Fast GC and Ultra Fast GC/MS for the Analysis of Essential Oils

11.45 L-02 **C. Bicchi**, C. Cordero, E. Liberto, P. Rubiolo, and B. Sgorbini, Turin, Italy
Headspace solid-phase dynamic extraction (HS-SPDE) for the analysis of the volatile fraction of matrices of vegetable origin

12.10 Lunch break

14.00 Plenary Lecture 2 Chair: Prof.Dr. A. C. Figueiredo

PL-2 **R. Naef**, Geneva, Switzerland
The complex chemistry of Camellia sinensis

14.50 L-03 **M. Kreck** and A. Mosandl, Frankfurt, Germany
Lilac Aldehyde and Lilac Alcohol – Bioconversion and Enantioselective Analysis of the Stereoisomers

15.15 L-04 T. Hashimoto, Y. Noma, and **Y. Asakawa**, Tokushima, Japan
Biotransformation of sesquiterpenoids from crude drugs and medicinal plants by microorganisms

15.40 L-05 **J.C.R. Demyttenaere**, J. Vanoverschelde, and N. De Kimpe, Ghent, Belgium
Monitoring of the bioconversion of (*R*)-(+)- and (*S*)-(−)-Citronellol by *Aspergillus* spp. and *Penicillium* spp. by SPME, SBSE and HSSE

16.05 Coffee break

Oral Communications Chair: Prof.Dr. G. Buchbauer

16.25 L-06 **N.A. Braun** and M. Meier, Holzminden, Germany
Western Australian and East Indian Sandalwood Oil – a Comparison

16.50 L-07 **S. Basar**, A. Koch, and W.A. König, Hamburg, Germany
Chemical Investigations on the Volatile Components of Olibanum Resins

L-08 **A.V. Tkachev**, Novosibirsk, Russia
Essential oils from Siberian plants: dependence of compositions on treatment procedures

17.40 L-09 **M.M. Barazandeh**, Tehran, Iran
Simplification of Retention Indices Calcuation by Upgrading GC Software

Tuesday September 9, 2003

9.00 Plenary Lecture 3 Chair: Prof.Dr. W. A. König

PL-3 **P. Schreier**, Würzburg, Germany
Progress in multi-element gas chromatography-isotope ratio mass spectrometry (HRGC-IRMS)

9.50 L-10 **W. Feger**, H. Brandauer, and H. Ziegler, Aufsess, Germany
Centrifugal Countercurrent Chromatography (CCC) In Citrus Oil Research

10.15 L-11 **D. Joulain**, Grasse, France
Analysis of "tree moss" extracts: an update

10.40 Coffee break

Oral Communicatons Chair: Prof.Dr. E. Stahl-Biskup

11.00 L-12 N.J. Ferreira, I.G.M. de Sousa, T.C. Luís, A.J.M. Currais, **A.C. Figueiredo**, P.A.G. Santos, J.G. Barroso, and L G. Pedro, Lisbon, Portugal
Pittosporum undulatum Vent.: Essential oil composition during capsule Maturation

11.25 L-13 M. Toyota, I. Omatsu, F. Nagashima, M. Murakami and **Y. Asakawa**, Tokushima, Japan
Sesqui- and diterpenoids and prenylbibenzyls from some New Zealand liverworts

11.50 L-14 **R.P. Adams**, Lorena, Texas, USA
Vetiver DNA fingerprinted cultivars: Effects of environment on growth, oil yields and composition

12.15 Lunch break

14.00 Plenary Lecture 4 Chair: Prof.Dr. H. Schilcher

PL-4 **R. Anton**, Strasbourg, France
Pharmacotoxicology and safety aspects of essential oils

14.50 L-15 **M. Tori**, Y. Takeichi, N. Morishita, K. Nakashima, and M. Sono, Tokushima, Japan
Chemical Constituents from *Eupatorium glehni*. A Comparative Study of Germacrane-type Sesquiterpenes from Different *E. glehni*

15.15 L-16 **F. Sefidkon**, R. Kalvandi, M. Atri, and M.M. Barazandeh, Tehran, Iran
Contribution for the characterization of *Thymus eriocalyx* chemotypes

15.40 Coffee break

16.00 -18.00 **Poster Session**

19.00 **Symposium dinner** (Residence palace)

Wednesday September 10, 2003

9.00 Plenary Lecture 5 Chair: Prof.Dr. Chl. Franz

PL-5 **W. Schwab**, Munich, Germany
Molecular biology: An indispensable tool for flavor research

9.50 L-17 **K. H.C. Baser**, F. Demirci, A. Pauli, Eskisehir, Turkey
Essential Oils and Components with Anticandidial Activity

10.15 L-18 **L. Jirovetz**, G. Buchbauer, Z. Denkova, A. Stoyanova, and I. Murgov, Vienna, Austria
Antimicrobial testings and chiral phase GC analysis of essential oils and aroma compounds

10.40 Coffee break

Oral Communications Chair: Prof.Dr. C.Bicchi

11.00 L-19 **J. Novak**, P. Mitteregger, P. Grassi, M. Skoula, C. Johnson, and C. Franz, Vienna, Austria
Does each essential oil gland on one leaf produce the same composition?

11.25 L-20 **O. Jansen,** C. Viallon, C. Raynaud, T. Talou, J.M. Bessière, and S. van Ruth, Toulouse, France
Black truffle aroma extracts: Identifying minor volatile compounds of high aroma impact

11.50 L-21 **S. Crane**, G. Aurore, P. Bourgeois, C. Raynaud, and T. Talou, Saint-Claude, France (Guadeloupe)
Volatile components from *Pouteria multiflora* (A. DC.) Eyma (Sapotaceae)

12.15 **Closing session**

12.45 Lunch break

14.30 **Excursion to Weikersheim Castle**

Abstracts
of Plenary Lectures

PL-1

Strategies for the Identification of known and unknown Essential Oil Constituents

Wilfried A. König[1], Detlev H. Hochmuth[2]

[1]Institut für Organische Chemie, Universität Hamburg, Martin-Luther-King-Platz 6, 20146 Hamburg, Germany;
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Only a small percentage of essential oil generating plants have been investigated so far. Although many of the volatile plant constituents are occurring in high redundance and can be easily identified by GC-MS there is always a certain number of compounds which can not be identified even by using the most efficient spectral libraries and data retrieving systems. These constituents may either be isomers of a family of compounds with similar or identical GC retention and mass spectral data or may be completely unknown. In the latter case isolation and investigation by NMR, IR and/or chemical conversion to a known compound is the method of choice for structure identification. Of course, it should be made sure that the constituents selected for isolation are really new. Nevertheless, the frustration of identifying a compound described before can not always be avoided. We have designed MassFinder [1], a software and data bank of (electron impact) mass spectra and retention indices (on a non-polar dimethylpolysiloxane stationary phase) for semi-automatic identification of known plant volatiles. This library presently contains ca. 1.800 entries and is constantly completed. It is particularly useful for the identification of the large majority of constituents in essential oils which have been identified before and have usually been described in the literature. It should be emphasized that the mass spectra of all compounds of the library were recorded under standard conditions on the same GC-MS instrumentation. All essential oil samples under investigation are run on the same instrument under identical conditions and "unknowns" can easily be filtered out and selected for further investigations.
For structure identification one- and two-dimensional NMR methods and mass spectrometry are the most efficient tools, while enantioselective GC in conjunction with chemical correlation (hydrogenation, dehydration, oxidation, rearrangement) is applied for deriving the absolute configuration of chiral plant constituents. Examples illustrating the unlimited diversity of metabolic pathways common to essential oil producing plants will be discussed.

[1] MassFinder 2.3: www.chemie.uni-hamburg.de/oc/koenig/massfinder.html

PL-2

The complex chemistry of tea (*Camellia sinensis* (L.) O. Kuntze)

Regula Naef

Firmenich SA, Corporate R&D Division, PO Box 239, CH-1211 Geneva 8, Switzerland

The chemistry of the leaves of *Camellia sinensis* which are the starting material for a great variety of teas will be reviewed. Very sophisticated processing steps lead to the specific teas by degradation of non-volatile compounds by enzymatic and non-enzymatic fermentation at different degrees which result in the characteristic tastes and aromas. The complexity of the tea flavour is due to an interaction of the polyphenols and caffeine with the volatile fraction. The formation of volatile flavour compounds depending on the treatment of the fresh tea leaves will be illustrated with some specialities of non-fermented (green), slightly fermented (white), fermented (black) and microbially fermented (red) teas and the constituents of fresh tea leaves will be presented.

PL-3

Progress in Multielement Gas Chromatography Isotope Ratio Mass Spectrometry (HRGC-IRMS)

P. Schreier, M. Appel, A. Hartlieb, S. Elss, F. Heckel, K. Hör, E. Richling, C. Ruff, and B. Weckerle

University of Würzbug, Faculty of Chemistry and Pharmacy, Chair of Food Chemistry, Am Hubland, D-97074 Würzburg, Germany

In authenticity studies of flavourings and essential oils, two principles, (i) enantioselectivity and (ii) isotope ratio, are used to control the origin of chiral and achiral volatiles, respectively. Whereas the fundamental studies of enantioselectivity go back to the beginning of the 1980s and nowadays well-established analytical techniques such as multidimensional gas chromatography (MDGC) and MDGC-mass spectrometry (MDGC-MS) are available, mass spectrometrical measurements of isotope ratios were limited to 'off-line' determinations of $^{13}C/^{12}C$ and $^{2}H/^{1}H$ ratios for a long time.

In the past decade, the on-line coupling of gas chromatography (HRGC) with isotope ratio mass spectrometry (IRMS) via a combustion interface (HRGC-C-IRMS) has opened the access to the analysis of $^{13}C/^{12}C$ ratios of individual constituents in complex natural matrices. Later, the measurement of $^{18}O/^{16}O$ ratios was made available in both 'off-line' and 'on-line' modes using pyrolysis (P) IRMS.

The large variations known to exist in the $^{2}H/^{1}H$ ratio in nature have made it an attractive target for IRMS studies and, recently, $^{2}H/^{1}H$ determinations of HRGC peaks became possible by P-IRMS using commercially available equipment.

Thus, at present, multielement HRGC-C/P-IRMS studies open new dimensions in authenticity evaluations. In the communication, the state-of-the art will be discussed by selected 'key compounds' originating from various plant sources.

The financial support provided by the FEI (Forschungskreis der Ernährungsindustrie, Bonn), the AiF and the Ministery of Economics (project no. 12969N) as well as the SAM GmbH, Mannheim, is gratefully acknowledged.

PL-4

Some pharmacotoxicological data and safety aspects of essential oils

Robert Anton

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A lot of essential oils are distributed in drugs, dietary supplements and cosmetics. Their worldwide consumption may lead to severe accidents because they contain lipophilic molecules such as terpene and phenylpropane derivatives. Consequently, these substances may have a high affinity for physiological human receptors and also negative side effects. As a consequence, a new risk assessment has to be developed by experts with the necessity to address following points :

- the parameters linked with the toxicological effects of essential oils;
- the consequences as far as toxicological data are concerned;
- clinical implications of both internal and external uses and the consequences of misuses;
- the answers given by national and European authorities in order to protect the consumer and to set limits of use;
- the recommendations concerning quality and a more precise labelling.

The lecturer will present this points of view and discuss the previously mentioned topics.

PL-5

Molecular biology: An indispensable tool for flavor research

W. Schwab

FG Biomolekulare Lebensmitteltechnologie, TU München, Lise-Meitner-Str. 34, D-85354 Freising, Germany
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In the last decade molecular biology methods have gained enormous popularity and are now intensively applied in studies on the biosynthesis, metabolism and function of essential oils. Today PCR methods are widely used for cloning genes whose sequences are known or can be derived from a protein's partial amino acid sequence. If a gene of an unknown protein or gene sequence must be cloned, a cDNA library is prepared and deposited in a set of transformed host organisms, usually *E. coli*. Once enough sequence information about the desired gene or gene product is available, synthetic primers can be constructed, which allows the gene to be cloned from cDNA using PCR. PCR cloning is combined with the insertion of a restriction site for ligation into an expression vector. Competent cells are transformed with the vector and transcription of the gene and expression of the protein is switched on by adding an inducer. The obtained protein can be analyzed for enzymatic activity. This lecture will present the cloning and expression of several genes isolated from a strawberry fruit cDNA library. The cDNAs were selected due to homologies with genes already known to be involved in flavor formation. The biosynthesis, metabolism and function of the volatiles will be demonstrated.

Abstracts
of Oral Comunications

L-01

Ultra Fast GC and Ultra Fast GC/MS for the Analysis of Essential Oils

Luigi Mondello and Giovanni Dugo

Dipartimento Farmaco-Chimico, Facoltà di Farmacia, Università di Messina, Viale Annunziata, I-98168 Messina, Italy

Conventional capillary GC has been, until recently, the prime technique for the analysis of complex natural matrices such as essential oils. The time required for a complete separation of all compounds of interest can, sometimes, be an hour or even more. The reason is due to the utilization of long capillary columns with 0.25/0.32 mm internal diamaters and slow temperature program rates. The increasing replacement of conventional methods with Ultra-Fast GC has been the source of a substancial reduction in the time required for separation with minimum or no loss in resolution. Originally, the basic problem to resolve was that the parameters imposed by Ultra-Fast GC theory were too extreme for conventional instruments. Modern technology now allows the application of high inlet pressure and split flows, highly accelerated temperature ramps and fast acquisition rates. The utilization of narrow bore capillary columns,although characterized by the same phase ratios as many conventional columns, lead to the formation of sharper peaks. This is due to the fact that column band broadening is directly proportional to the i.d. while film thickness influence is neglectable. The use of hydrogen as the mobile phase permits higher than optimum velocities with little loss in plate height. The sum of the above factors makes high speed separations possible. The volatile fraction of a citrus essential oil contains several classes of compounds; the most important are monoterpene, sesquiterpene hydrocarbons and their oxygenated derivatives, alcohols, esters and aliphatic aldehydes. These substances have a key role in the formation of the olfactory properties that are unique for each essential oil. Therefore, the qualitative and quantitative determination of these compounds define quality and possible adulterations of an essential oil. Ultra-Fast GC separations were carried out on samples of bergamot, lime, sweet orange and lemon oils. We obtained an outstanding reduction in time by factors of ten or more, without affecting resolution.

L-02

Headspace solid-phase dynamic extraction (HS-SPDE) for the analysis of the volatile fraction of matrices of vegetable origin

Carlo Bicchi, Chiara Cordero, Erica Liberto, Patrizia Rubiolo, Barbara Sgorbini

Dipartimento di Scienza e Tecnologia del Farmaco, Università di Torino, Via Pietro Giuria 9, I-10125 Torino, Italy
carlo.bicchi@unito.it

Over the last ten years there has been a remarkable renewal of interest in headspace sampling, in particular because of the introduction of high concentration capacity techniques. The best known of such techniques are headspace solid-phase microextraction (HS-SPME) and high capacity headspace sorptive extraction (HSSE)
More recently, Chromtech (Idstein, Germany) introduced an inside-needle technique for vapour and liquid sampling. In Solid-Phase Dynamic Extraction (SPDE), also known as "the magic needle", analytes are concentrated on a 50 ìm film of polydimethylsiloxane (PDMS) and activated carbon (10%) coated onto the inside wall of the stainless steel needle (5 cm) of a 2.5 mL gas tight syringe. When used for HS-SPDE, a fixed volume of the headspace of the sample under investigation is sucked for a suitable number of times with the gas tight syringe and an analyte amount suitable for a reliable GC or GC-MS analysis accumulates in the polymer coating on the needle wall. This communication reports the preliminary results of both a study on the optimisation of sampling parameters conditioning HS-SPDE recovery through the analysis of a standard mixture of highly volatile compounds and of HS-SPDE-GC-MS analyses of aromatic plants and food samples.

L-03

Lilac Aldehyde and Lilac Alcohol – Bioconversion and Enantioselective Analysis of the Stereoisomers

Mirjam Kreck[1], Armin Mosandl[2]

[1]Forschungsanstalt Geisenheim, Fachgebiet Weinanalytik und Getränkeforschung, Rüdesheimer Str. 28, D-65366 Geisenheim, Germany

[2]Institut für Lebensmittelchemie, Biozentrum, J. W. Goethe-Universität, Marie-Curie-Str. 9, D-60439 Frankfurt/Main, Germany

M.Kreck@fa-gm.de

Lilac aldehyde and lilac alcohol have been described as characteristic monoterpenoids in *Syringa vulgaris* L. flowers, with a desirable influence on lilac flavour quality.
The enantioselective analysis of chiral flavour using multidimensional gas chromatography mass spectrometry (enantio-MDGC-MS) has proved to be an efficient and selective tool to evaluate the origin of the flavour.
Since enantio-MDGC-MS technique was connected to Stir Bar Sorptive Extraction (SBSE) – the latest extraction technique for organic analytes from aqueous samples – there was created the most efficient and selective analytical configuration for the online chirality evaluation of flavour compounds from complex matrices.
The chiral monoterpenoids lilac aldehyde and lilac alcohol were analysed by this new online-technique with regard to the bioconversion and structure elucidation of the naturally occurring stereoisomers.
Four diastereoisomers of 2-[(5′-methyl-5′vinyl)tetrahydrofuran-2′-yl]propanal and -propanol were assigned as the genuine structure of lilac aldehyde and lilac alcohol respectively. The biogenetic origin of these monoterpenoids in *Syringa* species was disclosed by feeding experiments with deuterated compounds assumed to be the precursors of lilac aldehyde or lilac alcohol.

Literature:

[1] Baltussen E, Sandra P, David F, Cramers C (1999) J Microcol Sep 11 : 737
[2] Wakayama S, Namba S, Hosor K, Ohno M (1973) Bull Soc Chem Jap 46 : 3183-3187
[3] Kreck M, Püschel S, Wüst M, Mosandl A (2002) J Agric Food Chem 51 : 463-469
[4] Kreck M, Mosandl A (2003) J Agric Food Chem 51 : 2722-2726

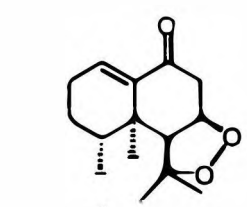
L-04

Biotransformation of sesquiterpenoids from crude drugs and medicinal plants by microorganisms

T. Hashimoto[1], Y. Noma[2] and Y. Asakawa[1]

[1]Faculty of Pharmaceutical Sciences, [2]Faculty of Human Life Sciences, Tokushima Bunri University, Yamashiro-cho, Tokushima 770-8514, Japan

The biotransformation of terpenoids from crude drugs and medicinal plants by microorganisms was carried out to obtain the functional substances (Hashimoto, Noma & Asakawa 2001; Hashimoto et al., 2002). Nardosinone (**1**), which shows antimalarial activity, from *Nardostachys chinensis* was biotransformed by *Aspergillus niger* for 1 day to afford the metabolites **2-5**. Biotrasformation of artemisinin (**6**) which also indicates antimalarial activity from *Artemisia annua* by *A. niger* gave compounds **7** and **8**. Maalioxide (**9**) and bicyclohumulenone (**13**) from the aromatic liverwort *Plagiochila sciophila* were biotransformed by the same fungus to yield compounds **10** and **11** from **9**, and compound **14** from **13**, respectively. Compound **9** was also converted to **12** by *A. cellulosae*. 2,3-Epoxide (**15**) of **13** was biotransformed by *A. niger* to afford compound **16.**



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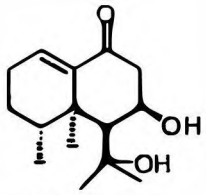

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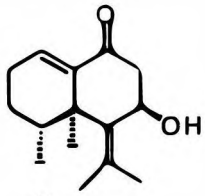

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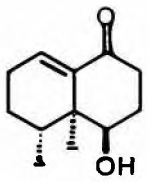

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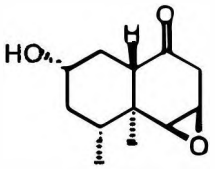

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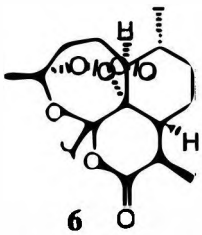

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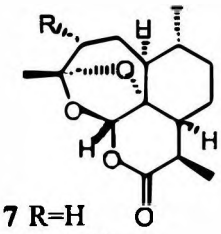
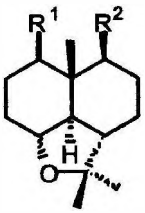
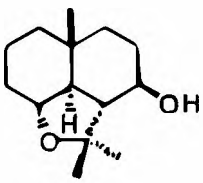


7 R=H
8 R=OH



9 R^1= R^2=H
10 R^1=OH, R^2=H
11 R^1=R^2=OH



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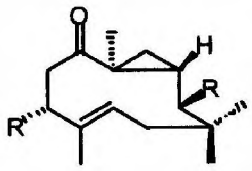
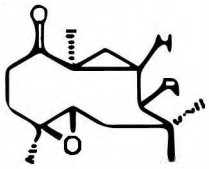


13 R=H
14 R=OH



15 R=H
16 R=OH

Their stereostructures were established by a combination of high-resolution NMR spectral and X-ray crystallographic analyses and chemical reaction. 1-Aminobenzotriazole, the inhibitor of cytochrome P-450, inhibited the oxidation process of these starting materials by *A. niger*.

Hashimoto, T., Noma, Y., Asakawa, Y. (2001) *Heterocycles*, 54, 529-559.

Hashimoto, T., Noma, Y., Nishimatsu, N., Ohnishi, S., Asakawa, Y. (2002), 33rd ISEO, Abstract. P. 34, Lisbon.

L-05

Monitoring of the bioconversion of (*R*)-(+)- and (*S*)-(−)-Citronellol by *Aspergillus* spp. and *Penicillium* spp. by SPME, SBSE and HSSE

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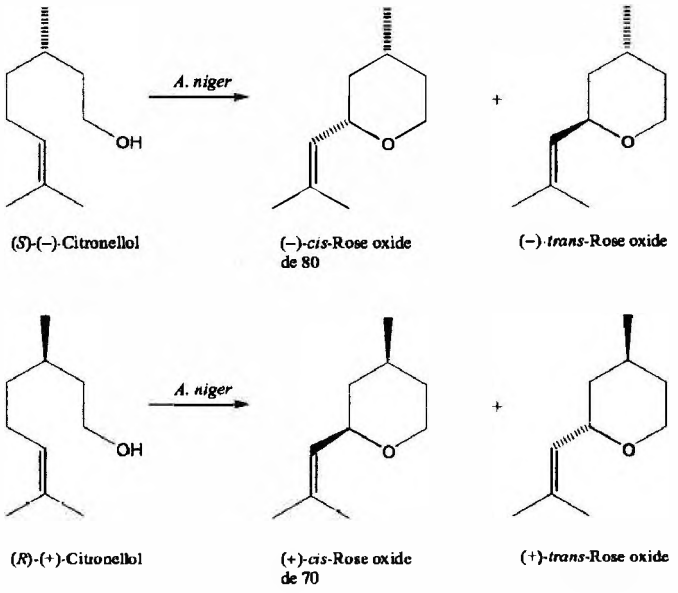
In the course of our work related to the biotransformation of monoterpene alcohols, aldehydes [1] and hydrocarbons [2], we studied the biotransformation of (*R*)-(+)- and (*S*)-(−)-citronellol by fungi. For screening experiments, solid phase microextraction (SPME) and stir bar sorptive extraction (SBSE), both in the liquid and headspace mode, *i.e.* headspace sorptive extraction (HSSE), were used as analytical techniques. It was found that sporulated surface cultures of *Aspergillus niger* were able to convert the substrate citronellol into *cis*- and *trans*-rose oxides and nerol oxide. The relative content in the headspace SPME extract of the three bioconversion products *cis*-rose oxide, *trans*-rose oxide and nerol oxide mounted to 54, 21 and 12%, respectively. Other bioconversion products were 6-methyl-5-hepten-2-one, 6-methyl-5-hepten-2-ol, limonene, terpinolene, linalool and α-terpineol. These bioconversion reactions were confirmed by sporulated surface cultures on larger scale and sampling by dynamic headspace on Tenax and steam distillation solvent extraction. The same conversions were noticed with *A. tubingensis* and *Penicillium roqueforti*. This bioconversion yielded more *cis*- than *trans*-rose oxide (*cis*/*trans* ratio up to 9/1; de 80). Submerged liquid cultures of *P. roqueforti* yielded two unidentified metabolites after conversion of citronellol (yield up to 5%). The stability and acid catalysed conversion of citronellol was also investigated. No chemical oxidation or auto-oxidation products were detected at ambient temperature in acidified liquid control broths up to pH 3.5. However, when control tests were run with solid media and when heat treatment (steam distillation solvent extraction) was applied, acid-catalysed conversions of the substrate to small amounts of *cis*- and *trans*-rose oxides, nerol oxide, linalool and α-terpineol were observed at pH 3.5.



[1] J.C.R. Demyttenaere, M.C. Herrera, N. De Kimpe, Phytochemistry 55 (2000) 363.
[2] J.C.R. Demyttenaere, K. Van Belleghem, N. De Kimpe, Phytochemistry 57 (2001) 199.

L-06

Western Australian and East Indian Sandalwood Oil – a Comparison

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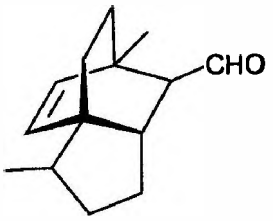
The sandalwood odor type is of great importance for the fragrance industry. This very pleasant note is achieved with synthetic sandalwood odorants and natural essential oils. Main sandalwood oil qualities on the market are of East Indian or Western Australian origin. These oils are produced from stem wood or roots of *Santalum album* L. and *Santalum spicatum* (R. Br.) A. DC. trees, respectively, by steam distillation or solvent extraction and subsequent steam or vacuum distillation.
East Indian sandalwood oil is favored by the perfumers and known in the flavor and fragrance industry as an excellent source for the search of new, odor active molecules. While East Indian sandalwood oil is very well investigated only little is known about its Western Australian counterpart. Could this oil really be the long searched substitute for the East Indian quality?
In this communication we report about the isolation and characterization of several new natural products from Western Australian sandalwood oil, e.g. nor-helifolenal isomers (**1**), present detailed analyses of both oils and a possibility – chiral GC analysis – to differentiate between the two Santalum species.



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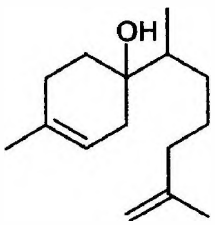

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In addition the isolation, total synthesis, and olfactory properties of iso-β-bisabolol (**2**), a new, odor active sesquiterpene from East Indian as well as Western Australian sandalwood oil will be discussed in detail.

L-07

Chemical Investigations on the Volatile Components of Olibanum Resins

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Olibanum is an oleogum resin that exudes from insicions in the bark of *Boswellia* species (Burseraceae). The trees yielding the resin are native to Ethiopia, Somalia, the Arabian peninsula and to India. *Boswellia carterii*, *Boswellia frereana*, *Boswellia papyrifera*, *Boswellia neglecta* and *Boswellia serrata* (India) are considered the most well known species [1].

In folk medicine olibanum has been used as a powerful anti-inflammatory and anti-arthritic agent since ancient times. Especially, the Indian traditional medicine, Ayurveda, has given olibanum an important role in the treatment of rheumatism, respiratory diseases and liver disorders. All these mentioned medical effects are attributed to the triterpenoic acids, particularly to the pentacyclic boswellic acids.

In addition to its use as a natural medicinal drug, olibanum and its oil have been used as an antiseptic agent, an ingredient in perfumery products and as an incense agent in churches.

In this study we compared the essential oils of five different *Boswellia* species; *B. carterii*, *B. serrata*, *B. frereana*, *B. neglecta* and *B. rivea* by TLC, GC and GC-MS. The diterpenoic constituents of these species were found to be diagnostic markers for species identification.

Secondly, the use of olibanum as an incense agent forced us to design a solid phase adsorption method for the analysis of the pyrolysis products formed on contact of the resins with burning charcoal. Differently from previous studies on the pyrolysis of olibanum [2,3] we think that our analytical approach is particularly close to the common usage conditions.

The interpretation of the results showed that new triterpenoic constituents are formed during pyrolysis of *B. carterii* and *B. serrata*. After the isolation and investigation of these constituents by 1- and 2-D NMR techniques they were identified as decarboxylation and dehydration products of the different boswellic acids. Some diterpene constituents and the triterpene tirucallic acid were found unchanged in the pyrolysis products. Biological activity studies on the pyrolysis products are in progress.

[1] Martinetz, D., Lohs, K., Janzen, J., " Weichrauch und Myrrhe", WVG, Stuttgart, 1988.

[2] Pailer, M., Scheidl, O., Gutwillinger, H., Klein, E., Obermann, H., *Monatshefte f. Chem.*, **112**, 314-358, 595-603, 987-1006, 1981.

[3] van Bergen, F.P., Peakman, T.M., Leigh-Fairbank, E.C., Evershed, R., *Tet. Lett.*, **38** (48), 8409-8412, 1997.

L-08

Essential oils from Siberian plants: dependence of compositions on treatment procedures

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Novosibirsk Institute of Organic Chemistry, Russia

Compositions of essential oils from different plants (*Asteraceae*, *Lamiaceae*, *Apiaceae*) growing wild in Altai region (Southern Siberia, Russia) have been studied by GC-MS. For all the plants investigated two types of essential oil samples were prepared: (1) the oil from fresh grass, (2) the oil from the dried grass. Obvious clear-cut general distinctions between these pairs of samples are as follows: (*i*) difference in content of low and high boiling fractions, (*ii*) difference in relative content of oxygenated (natural and artificial) derivatives, (*iii*) primary mobility of polyunsaturated conjugated olefins. All the plants studied can be divided in two groups according to constancy or inconstancy of composition of their essential oils. At the same time, these two groups differ in types of predominant secretory structures where essential oils are accumulated. Two types of secretorial structures are typical for the plant groups studied: the glandular trichomes and shizogenous cavities. Essential oils from the glands and trichomes are exposed to different processes to a variable degree. It is this set of processes (biochemical, chemical and physical) that affects the composition of essential oil during cutting of the plant, drying and storage processes. Peculiarities of the essential oil compositions and character of the dynamics of the main constituents as a function of predominant secretory structures are discussed.

L-09

Simplification of Retention Indices Calculation by Upgrading GC Software

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During researchs on aromatic plants of Iran,we had always a problem and it was the lack of a software for simple and fast calculation of gas chromatographic retention indices.So we had to use a scientific calculator to do that but in the case of many analyses it was a tedious and time consuming work.For solving this problem it was the first necessity that we replace the *Chromatopac C-R3A* data processor (Coupled to Shimadzu GC-9A) which was working under Dos (V1.2) with a new one which runs under Windows. We decided to joint GC to a HPLC (Knauer Model) interface box which was working under *Eurochrom 2000 for Windows* software.Then we wrote a computer program in basic language which calculates GC retention indices very fast and accurate only by exporting the peak report table of analysis and using it in the program.After that many analyses of essential oils have been done and it was shown many facilities which resulted in working under windows and also fast and accurate calculation of retention indices.

L-10

Centrifugal Countercurrent Chromatography (CCC) in Citrus Oil Research

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High Speed Countercurrent Chromatography (HS-CCC) constitutes a liquid-liquid chromatographic method where both, stationary and mobile phase, are (imiscible) solvents. As no solid is used as solvent-carrier, CCC can be carried out in normal-phase or reversed-phase modus.

Preparative scale CCC was applied to citrus oils and optimized for cold pressed oils of Key and Persian limes. The non-volatile part of these lime oils, which contain coumarins and psoralens, were separated and characterized by GC-MS and HPLC-DAD.

The main lime coumarins and psoralens (herniarin, citropten, isopimpinellin, bergapten, oxypeucedanin, bergamottin and 5-geranyloxy-7-methoxy-coumarin) could be isolated in amounts of 100 mg. A series of minor coumarins and psoralens, some of them were previously unknown in lime, were detected and identified.

Moreover some polymethoxyflavones, so far confirmed in orange, mandarin and grapefruit varieties, could be identified as trace components of lime oils.

L-11

Analysis of "tree moss" extracts: an update

Daniel Joulain

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Lichen extracts, referred to as *resinoids*, are used in perfume compounding for their fragrance value and so far unmatched fixative properties. Large amounts of two lichen species are used as raw materials for the perfume industry : as of 1997, a total of *ca.* 1900 tons/year of *Evernia prunastri* ("oak moss") and *Pseudevernia furfuracea* (L.). Zopf (so-called "tree moss") were processed, mainly at Grasse, France. When growing on pine trees, "tree moss" is a heterogeneous raw material made of lichen and elements from the host plant, viz. wood, twigs, bark etc. The chemical composition of tree moss has been thoroughly investigated by Tabacchi *et al.* [1) 2)], starting from the lichen itself and typical industrial extracts. This generated mainly qualitative data, which are reported in Huneck and Yoshimura's compilation [3)]. However, due to the variety and complexity of the manufacturing processes, very little is known on the quantitative composition of tree moss industrial extracts and the absolutes derived from them. Recent issues concerning the skin sensitising properties of lichen resinoids have prompted us to investigate the quantitative composition of tree moss extracts. We report herein a detailed analysis of tree moss as a raw material, as well as of the corresponding extracts. While atranorin and chloroatranorin were quantified by reversed phase HPLC, other lichen substances (monocyclic aromatic compounds, depsides, depsidones etc.) were most conveniently detected and quantified by GC-MS with an internal standard after TMS derivatization. Triterpenols like β-sitosterol were analyzed by HPLC fitted with an evaporative light scattering detector (ELSD). Terpenoids, including resinic acids, are present in the host plant (*Pinus spp.*). Dehydroabietic acid (DHA), one of the main components of the resinic acids, was quantified by HPLC with fluorimetric detection, whereas 7-oxodehydroabietic acid (7-oxoDHA) was preferably quantified by GC-MS, either as the TMS derivative or as the methyl ester. In the latter case, methylation was achieved with diazomethane, and methyl-d_3 7-oxo-dehydroabietate **4** was the added internal standard. Following previous observations by Tabacchi [2)], our results confirm that 1) diterpenic acids which are biosynthetized in the host plant migrate into the lichen and 2) the lichen participates in the conversion of some of them into oxidized species.

Concerning the alleged skin sensitising properties of tree moss extract, we report data which suggest that the main culprits are indeed the oxidized resinic acid, rather than depsidic compounds present in the lichen.

For the first time, carbon, hydrogen and oxygen Stable Isotope Ratio Analysis (SIRA) and NMR site specific deuterium analysis could be used to confirm some biosynthetic pathways for the formation of monocyclic aromatic lichen substances. These measurements can be used for the assessment of the origin of major components in lichen extracts.

1) J. Gunzinger, *Thesis*, University of Neuchâtel, Switzerland (1985).
2) R. Tabacchi, G. Tsoupras, in: *Progress in Terpene Chemistry* (D. Joulain, Editor), Editions Frontières, 293-305 (1986).
3) S. Huneck, I. Yoshimura, *Identification of Lichen Substances*, Springer Verlag (1996).

L-12

Pittosporum undulatum Vent.: Essential oil composition during capsule maturation

Nicolau J. Ferreira, Inês G. Meireles de Sousa, Tiago Cunha Luís, António José M. Currais, A. Cristina Figueiredo, Pedro A. G. Santos, José G. Barroso, Luis G. Pedro

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Pittosporum undulatum is a large evergreen tree, native of southeast Australia. This ornamental temperate/sub-tropical tree was the most commonly grown of the Australian pittospora, but it is now declared weed on all continents (Cayzer *et al.* 2002). The fruits are nearly globular capsules (ca. 12 mm across) that take about 6-8 months to mature. These capsules possess two to three thick coriaceous valves and usually contain 20-40 sticky bright orange seeds, which are bird-dispersed. The name *Pittosporum* derives from two Greek words, meaning, "pitch" and "seed," referring to the stickiness of the seeds.

The fruits of *P. undulatum* were collected fortnightly during eight months from non-pruned trees grown at the Parque de Saúde de Lisboa. During the collection period, the fruits evolved macroscopically through three main stages of development, green capsules (GC), orange capsules OC) and dehiscent capsules (DC). The essential oils were isolated from deep-frozen fruits by hydrodistillation to estimate the oil yields, and by distillation-extraction, to determine their percentage composition, and analysed by GC and GC-MS.

The essential oils isolated from *P. undulatum* fruits were obtained in yields ranging from 0.23% to 0.75% (v/w). The average oil yield from the fruits (0.42%) was 5.7 fold higher than the average of the corresponding leaf oil yield (0.073%) (Ferreira *et al.* 2002).

In common with the previous study on the essential oil from the leaves (Ferreira *et al.* 2002), monoterpenes were dominant in all oils (>87%), the monoterpene hydrocarbons constituting always the main fraction (>67%). Sabinene (32-52%), limonene (12-30%) and terpinen-4-ol (4-17%) were the major components of the oils, although with some variations in their relative amount during capsule maturation.

Sesquiterpenes occurred in a relative amount <9%, and bicyclogermacrene was, as in the previous leaf essential oil study (Ferreira *et al.* 2002), the dominant component of this fraction, in a relative amount <5%. A third fraction of non-terpenic compounds attained a relative amount <0.5% of the total oil.

Acknowledgements: The authors gratefully acknowledge the permission of the Parque de Saúde de Lisboa for collection of plant material.

Cayzer L. W., M. D. Crisp, I. R. H. Telford (2000) Revision of *Pittosporum* (Pittosporaceae) in Australia, *Australian Systematic Bot.* 13: 845-902.

Ferreira N. J., I. G. Meireles de Sousa, T. Cunha Luís, A. J. M. Currais, A. C. Figueiredo, J. G. Barroso, L. G. Pedro (2002) Seasonal variation of the leaf essential oil from two populations of *Pittosporum undulatum* Vent. grown in the Portuguese mainland, *33rd International Symposium on Essential Oils*, Portugal, [Abstract] p. 74.

L-13

Sesqui- and diterpenoids and prenylbibenzyls from some New Zealand liverworts

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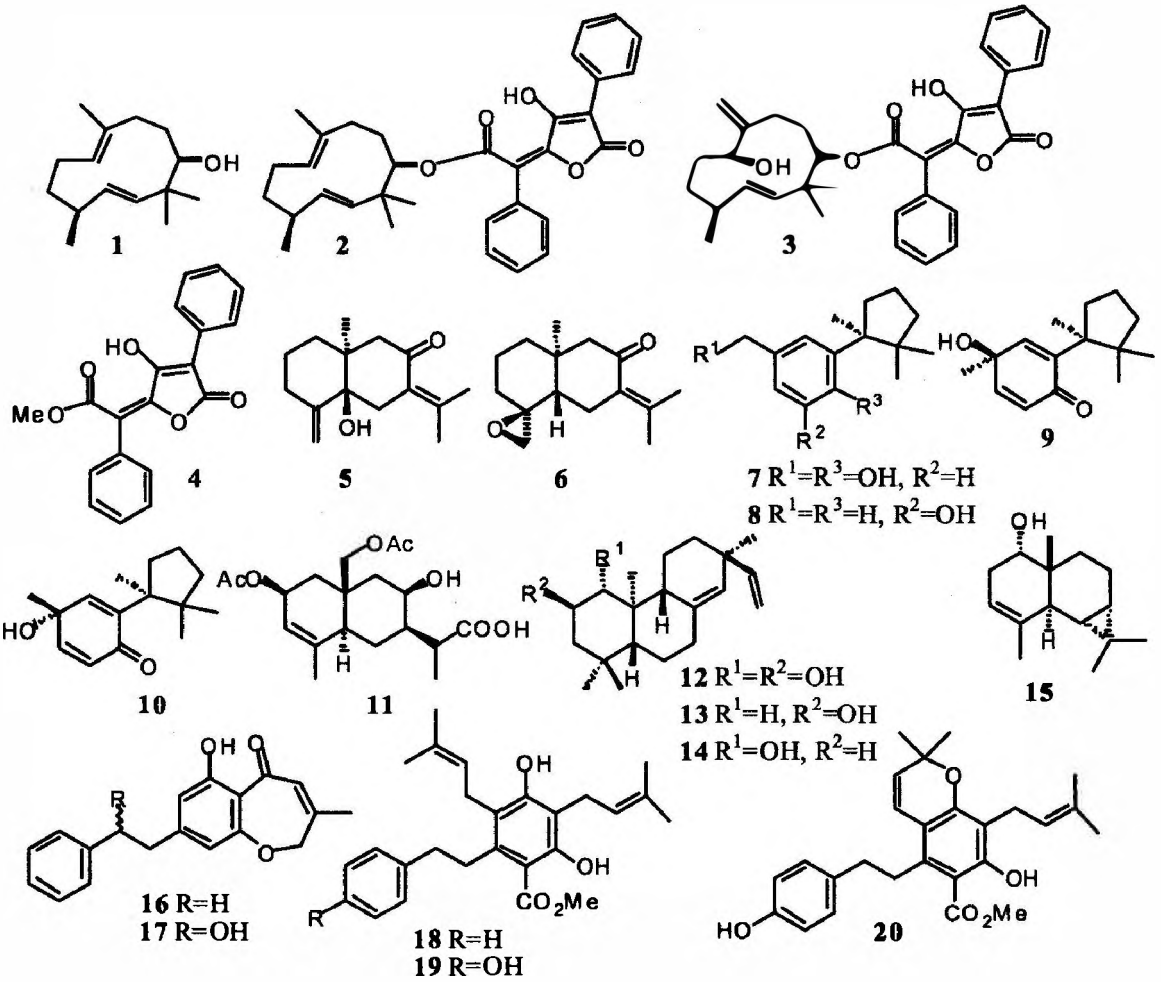
We are continuing to study the biologically active constituents of southern hemispheric liverworts (Nagashima et al., 1999; Asakawa 2000; Asakawa et al., 2003, Bardon et al., 1999, 2000). The ether extracts of New Zealand *Tylimanthus tenellus, Chiloscyphus, Herbertus* (?), *Heteroscyphus* species, *Trichocolea mollissima* and *Marsupidium epiphytum* were fractionated to give three new sesquiterpenoids (**1-3**), *ent*-α- and β-selinenes and vulpinic acid (=methyl pulvinate)(**4**) (from *T. tenellus*), two *ent*-cyclogermacrones (**5,6**) with *ent*-α- and β-cyclogermacrones (*Chiloscyphus* sp.), two new herbertenols (**7,8**), with two known herbertenones (**9,10**) (*Herbertus* sp. ?), a new *ent*-maaliene- (**11**) (*Heteroscyphus* sp.), a new eudesmane-type sesquiterpenoids (**11**) and 5 new prenylbibenzyls (**16-20**)(*Marsupidium epiphytum*) and two new *ent*-pimaranes (**12,13**) with the known *ent*-pimarane (**14**). The structures of newly isolated compounds were elucidated by ^{1}H- and ^{13}C-NMR spectral and X-ray crystallographic analyses. The isolation and the structure determination of the new compounds and chemosystematics of these liverwort species will be discussed.



Asakawa, Y. (2001) *Phytochemistry* **56**, 297-312.
Asakawa, Y., Toyota, M., von Konrat, M, Braggins, J. E. (2003) *Phytochemistry* **62**, 439-452.
Bardon, A., Kamiya, N., Toyota, M. Asakawa, Y. (1999) *Phytochemistry* **51**, 281-287.
Bardon, A., Mitre, G. B., Kamiya, N., Toyota, M., Asakawa, Y. (2002) *Phytochemistry* **59**, 205-213.
Nagashima, F., Murakami, Y., Asakawa, Y. (1999). *Phytochemistry* **51**, 1101-1104.

L-14

Vetiver DNA fingerprinted cultivars: Effects of environment on growth, oil yields and composition

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Twenty one accessions of vetiver (*Vetiveria zizanioides* (L.) Nash, sterile, oil type) and Khus (*V. zizanioides,* fertile, non-oil type) were analyzed by the use of random amplified polymorphic DNAs (RAPDs). Nineteen of the accessions clustered strongly around the cultigen, Sunshine. Three accessions, Khus, Northern India, Kassel, Germany, and Guang Dong, China clustered loosely and were not closely related to the sterile oil producing vetivers. Thirteen of the vetiver accessions were grown in test plots in Florida, USA, Nepal and Portugal. The largest growth was recorded in Nepal, followed closely by Florida and by the cooler, Mediterranean site in Portugal. No single genotype (DNA cultivar) grew best in every plot. Oil yields (% oil/dry wt.) were highest in Nepal and Portugal. Oil yields ranged from 0.29% to 9.61%. Essential oil production (g/plant) was highest in Nepal and Florida and ranged from 0.02 to 4.17 (g/plant). Analyses of variation among the major compounds is discussed.

L-15

Chemical Constituents from *Eupatorium glehni*. A Comparative Study of Germacrane-type Sesquiterpenes from Different *E. glehni*

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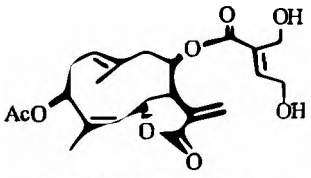
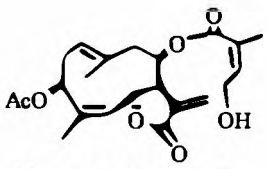
Chemical constituents of *Eupatorium glehni* collected in Hokkaido, Tokushima and Nagano in Japan were investigated. All produced germacrane-type sesquiterpenes with different esters at C-3 or 8 positions. Those from Nagano Prefecture afforded hiyodorilactones A, B, C, and D, and others (**1-6**), which are highly oxygenated with 4,5-*cis* double bonds. However, those from Hokkaido and Tokushima were less oxygenated and some have 4,5-*trans* double bonds (**7-9**). This plant was used to be called "*E. sachalinense*", but now the name should be changed to "*E. glehni*" as pointed out by Kawahara. The discrepancies of these findings may be attributed to the difference in the places, although we do not know if this is due to the difference in the races. We are going to work in this area in the future.



hiyodorilactone A (**1**)



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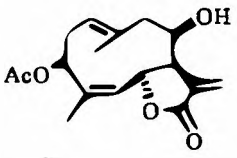
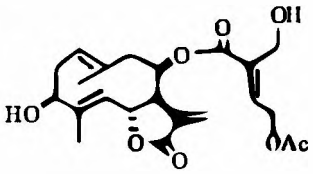
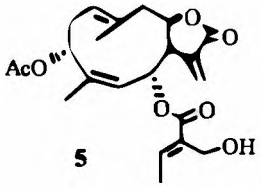


hiyodorilactone C (**3**)



hiyodorilactone D (**4**)



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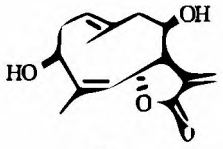

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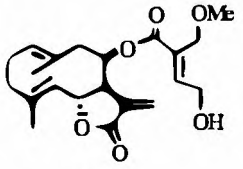

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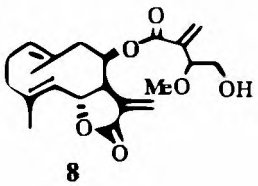

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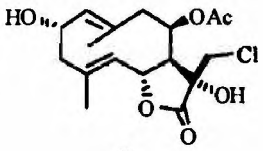

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We thank Dr. T. Kawahara for identification of the plant.

L-16

Contribution for the characterization of *Thymus eriocalyx* chemotypes

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Essential oils were obtained by hydro-distillation from the aerial parts of *Thymus eriocalyx* (Ronniger) Jalas, at full flowering stage, from various locations in central and west Iran. Gas chromatography and gas chromatography/mass spectroscopy analyses of the oils revealed that the major components linalool (1.8%-60.4%), geraniol (trace-50.5%), and thymol (1.6%-58.4%) varied widely. Based on the variation in oil composition between the various taxa, the existence of three chemotypes is proposed.

L-17

Essential Oils and Components with Anticandidial Activity

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Some of the yeasts occur ubiquitous and they belong to the normal flora of humans. Many species are without any clinical significance, but some yeast are regarded as opportunistic pathogens, that can cause infections especially in debilitated patients. *Candida* is one of the important genera among yeasts, which includes human pathogenic species *C. albicans* or *C. krusei*. Normally yeasts live in balance with other bacteria and yeast, however, abnormal conditions can cause them to multiply followed by a systemic infection. Candidiasis can range from superficial disorders such as diaper rash to invasive, rapidly fatal infections in immunocompromised cases.

Essential oils are well known and used for their antimicrobial effects for ages by mankind. Essential oils and their constituents such as monoterpenes, sesquiterpenes, diterpenes, aromatic, aliphatic substances etc. have shown remarkable activity against *Candida* comparable to those of conventional antifungal agents. In this review, we report on the essential oils and groups of selected substances thereof - with evident anticandidial activity - which are promising candidates for further pharmacological studies.

L-18

Antimicrobial testings and chiral phase GC analysis of essential oils and aroma compounds

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As general known, enantiomeric properties of aroma compounds are of essential importance for their odor-impressions as well as for their biological activities. Therefore, an international cooperation has been started to test the antimicrobial effects of essential oils and pure aroma compounds and to analyze the tested samples for their enantiomeric purity of the target compounds by means of chiral phase GC. The combined interpretation of biological and analytical data should give valuable informations, if the chirality of odor-active components leads to a distinct difference in the antimicrobial effects.

The samples investigated are as follows: essential oils of lavender and dill as well as the aroma compounds (R)-(+)-camphor, (S)-(-)-camphor, racemic camphor, (R)-(+)-limonene, (S)-(-)-limonene, (-)-linalool, natural linalool, synthetic linalool, synthetic linalyl acetate, (+)-2-carene, (+)-3-carene, (S)-carvone, (R)-carvone, synthetic carvone, 1,8-cineole, eugenol and ß-caryophyllene. The enantiomeric properties of the target compounds were analyzed by GC-FID and GC-MS using cyclodextrin phases. The microorganisms *Staphylococcus aureus*, *Escherichia coli*, *Pseudomonas aeruginosa*, *Klebsiella pneumoniae* and *Candida albicans* were taken to test the antimicrobial activities (Agar Diffusion Cup Method and/or Agar Diffusion Disc Method) of the essential oils and aroma compounds.

The focus of this lecture will be set on some interesting as well as surprising results from combined data interpretations.

L-19

Does each essential oil gland on one leaf produce the same composition?

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SPME sampling of individual oil glands (1) has been used to measure the variation in genuine volatile content and composition in and within different oregano plants as affected by age, season and developmental state. The main monoterpenes found were *p*-cymene, carvacrol and their precursor γ–terpinene. The early season preponderance of *p*-cymene over carvacrol is reversed as the season progresses and this pattern can also be seen at any time within the plant, from the youngest to the oldest leaves. Within individual leaves this pattern was not observed, even within the youngest developing leaves. However it was found that the oil composition of individual glands within a single leaf varied considerably, most notably in respect of the production of carvacrol and its isomer thymol.

1. Kubezka K-H. 1997. New approaches in essential oil analysis using polymer coated silica fibers. in: Franz, Ch.; Máthé Á.; Buchbauer G. Essential Oils: Basic and Applied Research. *Proceedings of the 27th International Symposium on Essential Oils, Allured Publishing Corpration, Carol Steam, IL*; 139-146.

L-20

Black truffle aroma extracts: Identifying minor volatile compounds of high aroma impact

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The odour-active compounds of the Black truffle (*Tuber melanosporum* Vitt.) have been subject of analytical studies since the early 1980ies, leading to a patented formula comprising 9 compounds. While these major, low-boiling-point aroma constituents make up for more than 95 percent of the mushroom's headspace volatiles, little is known about the contribution of minor, less volatile odourants. As the latter tend to fall below the instrumental detection threshold, emphasis was put on spotting them by GC-olfactometry (GC-O). In these experiments, 10 additional odour peaks were found, all with relatively long retention times and lacking instrumental detection.
Further on, two different extraction techniques were subsequently used to concentrate these aroma constituents and to proceed to their identification. As a first technique, an industrial high-pressure steam cooking process was applied, leading to two different aqueous aroma extracts (one liquid, one viscous). The extracts' headspace was re-scanned for odourants by means of GC-O analysis with 2 panels consisting of 8-9 assessors each. To overcome the problem of low aroma release rates into the headspace, VOCs were then further concentrated by solvent extraction, using the simultaneous distillation-extraction (SDE) process. GC-O experiments were repeated on these extracts with syringe injection. Parallel GC-MS analysis allowed compound identification.

L-21

Volatile components from *Pouteria multiflora* (A. DC.) Eyma (Sapotaceae)

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Pouteria multiflora fruits were commonly used in the West Indies countries. They were well known as a source of pleasant aromatic fragrance despite the chemical aromatic compounds were not yet identified. Fresh and air-dried pulp, and seeds of *Pouteria multiflora* (A. DC.) Eyma were hydrodistillated. Complementary solvent extractions (methylene chloride) were performed on the different samples. The different extracts obtained were analysed by Gas Chromatography (GC) and High Resolution Gas Chromatography coupled with Mass Spectrometry (HRGC/MS). Chemical identifications were performed by computerized matching with mass data banks (WILEY, NIST...). Qualitative and quantitative differences were reported for the first time between the different aromatic extracts.

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P-01

Determination of the Absolute Configuration of a new Sesquiterpenoid and analysis of the Essential oil of the Liverwort *Plagiochila alsplenioides*

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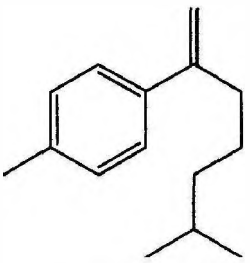
The essential oil of *Plagiochila alsplenioides* was prepared by hydrodistillation and analysed by GC and GC-MS. All known constituents were identified by mass spectrometry in conjunction with their gas chromatographic retention indices by comparison with a spectral library established under identical experimental conditions (Joulain and König, 1998; MassFinder software and data bank, Hochmuth et al. 2002). The two new compounds bisabola-1, 3, 5, 7(14)-tetraene (1) and muurolan-4, 7-oxide (2) were isolated by preparative-GC, -TLC etc. Their structural elucidation was achieved by chemical and physicochemical methods using mass spectrometry and 1- and 2D-NMR techniques. The absolute configuration of compound (2) was determined by chemical correlations (hydrogenation and rearrangement reactions) using enantioselective GC.



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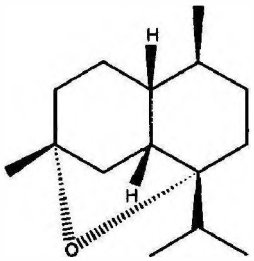

2

[1] Hochmuth, D. H., Joulain, D., König, W. A. 2002. MassFinder software and data bank, University of Hamburg (www.chemie.uni-hamburg.de/oc/koenig/massfinder.html).

[2] Joulain, D., König, W. A., 1998. *The Atlas of Spectral Data of Sesquiterpene Hydrocarbons*. E. B.-Verlag, Hamburg.

P-02

Volatile Oils of *Anthemis talyshensis* A. Fedor. and *Sclerorhachis platyrachis* (Boiss.) podlech ex Rech. f. from Iran

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Thirty-nine species of the genus *Anthemis* are found in Iran, among which fifteen are endemic(1). Only a few reports on the analysis of essential oils of *Anthemis* species have been published. Two species of the genus *Sclerorhachis* are found in Iran, which are endemic, *S. platyrachis* and *S. leptoclada* and are widely distributed in Province of Khorassan, North-east of Iran (1). The water distilled volatile oils from aerial parts of *Anthemis talyshensis* A. Fedor. and *Sclerorhachis platyrachis* (Boiss.) Podlech ex Rech. f. two Compositae species, which are endemic to Iran, were analyzed by GC and GC/MS. α-Eudesmol (18.2%), borneol (13.3%), hexadecanoic acid (9.5%), γ-eudesmol (8.6%) and elemol (7.6%) were the predominant constituents of the oil of *Anthemis talyshensis.* The oil of *Sclerorhachis platyrachis* consisted mainly of monoterpenes and a small percentage of sesquiterpenes. The major components found in the oil were α-pinene (31.2%), camphor (24.8%) and β-pinene (14.7%).

1. K.H. Rechinger, *Anthemis* and *Sclerorhachis*, In: *Flora Iranica*, Compositae No. 158. Edits., K.H.Rechinger and I.C.Hedge, pp. 26, 47, Akademische Druck and Verlags-anstalt, Graz, Austria (1986).

P-03

The Essential Oil and Polyacetylenes from *Eryngium yuccifolium* Michx. (Apiaceae)

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Continuing our investigations on essential oils belonging to the Apiaceae, especially from the genus *Eryngium*, we have analysed the essential oil of *Eryngium yuccifolium*, a plant native in the South of the United States from Connecticut to Florida, west to Minnesota, Kansas and Texas.

We have analysed the essential oil of plants cultivated in the medicinal plant growing area of Dr. Willmar Schwabe Company near Karlsruhe, south Germany. The oil was obtained from different parts of *E. yuccifolium* by hydrodistillation and analysed by GC, GC-MS and NMR spectroscopy, exhibiting quite different compositions in the leaves, stalks and the roots. In the leaves mono- and sesquiterpene hydrocarbons were the most abundant constituents with germacrene d (18.3%), terpinolene (17.8%), bicyclogermacrene (8.8%), α-pinene (7.6%), and ß-caryophyllene (6.2%) being the most prominent constituents. In addition, relatively high concentrations of the polyacetylene derivative falcarinol (9.6%) were detected.

In the stalks above all high amounts of germacrene d (38.4%), γ-amorphene (12.2%), and bicyclogermacrene (10.1%) besides smaller amounts of bicyclosesquiphellandrene (3.4%) and falcarinol (3.2%) were found.

The root oil from *Eryngium yuccifolium* differed significantly from the oils of the above ground green parts. Main constituents are terpinolene (25.8 %), *trans*-β-bergamotene (18.6 %) and the two benzaldehyde derivatives 2,3,6- and 2,3,4-trimethylbenzaldehyde (13.9 and 1.3%, respectively) which have to be considered as artifacts formed during hydrodistillation from ferulol and isoferulol esters by hydrolysis and proton-catalysed rearrangement as described earlier (1).

Surprisingly no polyacetylene derivative was detected in the essential oil from the roots, which are common constituents of *Eryngium* roots (2-5) and therefore we decided to investigate the hexane-ether extract (1:1) by TLC, MS and NMR spectroscopy resulting in the detection of some common polyacetylenes and a new constituent from this chemical class.

1. Kubeczka K.H. and Ullmann I., (1981) *Phytochemistry* ***20***, 828-830.
2. Bohlmann, F. and Zdero, C. (1971) *Chem. Ber.* **104**, 1957-1961.
3. Kubeczka, K.H., Ayoub, N., Grande, M., and Torres, P. (1998) Composition of the essential oils from different parts of *Eryngium maritimum* L. (Apiaceae), Poster presented at 29th International Symposium on Essential Oils, Frankfurt, Germany, 6-9.9.1998.
4. Kubeczka, K.H. , Ayoub, N., Nawwar, M., and Saleh, M. (1999) The essential oil and polyacetylens from *Eryngium campestre* L. (Apiaceae), Poster presented at 30th International Symposium on Essential Oils, Leipzig, Germany, 6-9.9.1999.
5. Ayoub , N. and Kubeczka, K.H. (2001) Composition of essential oils from *Eryngium amethystinum*, *E. alpinum* and *E. planum* (Apiaceae), Poster presented at 32nd International Symposium on Essential Oils, Wroclaw, Poland, 10-13.9.2001.

P-04

Chemical composition of the Essential Oil of *Camphorosma monspeliacum* L. from Iran

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The essential oil obtained by hydro-distillation (clevenger) from aerial parts of *Camphorosma monspeliacum* L. (Chenopodiaceae) was examined by GC and GC/MS. The yield of total volatile was 1.5 % (w/w.) A total of thirty-two compounds were characterized representing of about 85% of the total components detected. Based on the analysis of essential oil, the components were classified in four groups. The oil was characterized by a high content of alcohols which composed 35% of the oil. The major components were α-cadinol (9.1%), 1-octen-3-ol (8.2%), ß-eudosmol (7.3%), ß-bisabolene (6.1%), 2-tridecanone (5.1%), ß-cubebene (3.4%), neryl acetate (3.0%). Other compounds present in apreciable amounts are decanol (2.6%), thymol (2.2%), α-terpinol (2.1%), nonanal (2.0%), decanal (1.9%), pinocarvone (1.7%), pinocarveol (1.5%), limonene (1.3%) and geranyl acetate (1.2%).

References

1. Mozaffarian V. *A Dictionary of Iranian Plant names*, Farhang Moaser, Tehran, 1996, p 407.
2. Hooker J D and Jackson B D. *Index Kewensis*, Oxford at the Clarendon Press, 1960, vol **1**
3. Zargari A. *Medicinal plants*, Tehran University publisher, 1990, **4,** p 150
4. Sandra Pand, Bicchi C. *Capilary Gas Chromatography in Essential Oil Analysis,* Alfred Huethig Verlag: New York, 1987.
5. Alexandrina M., Chifu T., Davidescu G., Bireescu L., Geanina B and Rodica E. *The influence of the soil salinity on some physiological processes of the lawn plants from the Prut meadow*, Analele- Siintifice- ale- Universitatii-Al-I-Cuza-din-Iasi-Sectiunea-II-a.-Biologie-Vegetala, 1998, 44: 45-55.

P-05

Essential oil composition from the aerial parts of *Sideritis hirsuta* L. from Spain

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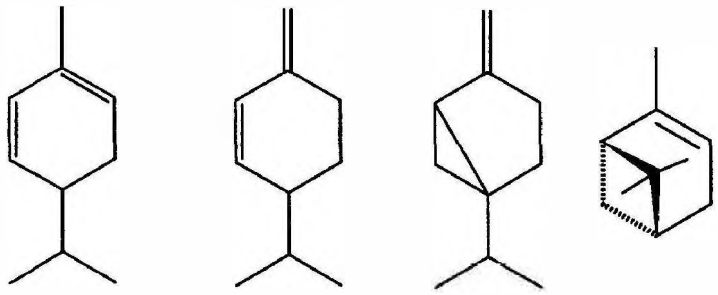
The genus *Sideritis* L. belongs to the Lamiaceae family, one of the most famous for the many plants which produce flavouring substances and culinary herbs in use throughout the ages. Twenty two of the twenty eight species described in Flora Eurpoaea grow wildly in Spain, including *Sideritis hirsuta* L. (1).

The essential oil from the aerial parts of *Sideritis hirsuta* L. has been extracted by steam distillation and analysed by Gas Chromatography (GC) and Gas Chromatography coupled to Mass Spectrometry (GC-MS). The monoterpenoid fraction was higher than the sesquitepenoid one. The principal constituents have been identified as β-phellandrene (32.3%), α-phellandrene (13.1%) and α-pinene (11.6%) and they amount more than the 50% of the total oil.

Main constituents



α-phellandrene β-phellandrene sabinene α-pinene

1. Flora Europaea, Vol. 3., Edited by T. G. Tutin, V. H. Heywood, N. A. Burges, D. H. Valentine, S. M. Walters and D.A. Webb, Cambridge at the University Press (1972).

P-06

Essential Oils Composition of the four Aromatic Plants from Iran

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Thymus fallax Fisch. & C.A. Mey[1] was collected from Hamedan (Hamedan province) in May 2002 and its dry leaves were hydrodistilled for 2 hrs. in a clevenger type apparatus to produce a light yellow oil at the yield of 2.5% (based on dry leaves).
Salvia hydrangea DC. ex Benth.[1] was collected from Esfahan (Esfahan province) in June 2002. Dry flowers of the plant were hydrodistilled for 2hrs. in a clevenger type apparatus to produce a light yellow thin layer of essential oil at the yield of 0.2% (based on dry weight).
Tanacetum polycephalum Schultz-Bip.[1] was collected from Lar-Lacem valley in June 2002 and its dry flowers were hydrodistilled for 3hrs. to produce an oil at the yield of 0.7% (based on dry weight).
Geranium rotundifolium L.[1] was collected from National Botanical Garden of Iran (Tehran) in June 2002 and 46 grams of its dry leaves were hydrodistilled in the phytochemistry lab. Because of low yield, the oil was separated from the aqueous phase by adding diethylether.
The four essential oils were analysed by GC and GC/MS:
Twenty-three compounds were identified in the essential oil of *T. fallax* among which thymol (65.9%) and ã-terpinene (10.8%) are the major constituents, respectively.
Twenty-eight compounds were identified in the essential oil of *S. hydrangea* among which â-caryophyllene (33.4%) and caryophyllene oxide (25.4%) have the highest percentages.
Among the thirty compounds in the essential oil of *T. polycephalum* camphor (46.3%), borneol (15.0%),1,8-cineole (9.0%), camphene (7.9%) and isobornyl acetate (4.9%) are the major constituents, respectivly.
Forty-two compounds identified in *G. rotundifolium* among which á-terpinyl acetate (39.3%) and pulegone (27.7%) have the highest percentages.

Reference:

1. V. Mozaffarian. *A Dictionary of Iranian Plant Names.* Farhang-e-Moaser Publishers (1996).

P-07

Essential Oils Composition of the three *Origanum* Species from Iran

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Three species of *Origanum (O. vulgare* L., *O. majorana* L. and *O. viride* (Boiss) Halacsy)[1] were collected from their growing locals for identification of their essential oils composition:
O. vulgare L. was collected from National Botanical Garden of Iran (located in Tehran-Karaj Highway) in Aug. 2002. Its dry flowers was steam-distilled for 45 min. in an all-glass apparatus. A light-yellow oil was produced at the yield of 0.3% (based on dry weight).
O. majorana L.(cultd.) was collected from National Botanical Garden of Iran in Aug. 2002 and 100gr. of its dry flowers were steam-distilled for 45 min. to produce a light-yellow oil at the yield of 0.3%.
O. viride (Boiss) Halacsy was collected from Chalus-Marzan Abad road (Height:50-80m) in July 2002. Dry flowers and leaves were steam distilled separately. The oils were produced at the yields of 0.4% and 0.2%, respectively.
All of the essential oils were injected to CGC-FID and GC/MS for qualitave/ quantitave identifications.
Thirty-six compounds were identified in the essential oil of *O. vulgare* which represent 99.9% of total oil among which ß-caryophyllene (24.5%), germacrene-D (15.2%), trans-sabinene hydrate (9.0%), sabinene (6.0%), α-humulene (5.1%), valencene (4.3%) and (E)-ß-ocimene (4.2%) are the major constituents.
Twenty-four compounds were identified in the essential oil of *O. majorana* among which linalyl acetate (26.1%) and sabinene (12.0%) are the major constituents, respectively.
Thirty-nine compounds were identified in the essential oils of dry flowers and leaves of *O. viride* among which thymol (24.2%, 20.2%) and γ-terpinene (22.5%, 12.9%) have the highest concentrations, respectively.

Reference:

1. V.Mozaffarian. *A Dictionary of Iranian Plant Names.* Farhang-e-Moaser Publishers(1996).

P-08

GC-MS analysis of essential oil from leaves of *Peucedanum tauricum* Bieb.

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Peucedanum tauricum Bieb. is an endemic perennial plant from *Apiaceae* family, growing in Crimea and Romania [1]. Investigations of essential oil from fruit of this plant were recently performed [2], and in this essential oil unknown sesquiterpenoids as predominating compounds were found (investigation are in progress).
In present work leaves of *Peucedanum tauricum* Bieb. collected in Botanical Garden in Lublin (Poland) were investigated on the presence of essential oil.
Qualitative and quantitative analyses of essential oil components were performed by GC-MS with an ITS-40 mass spectrometer (Finnigan MAT, USA), MS 70 eV, 220 °C, GC-FID (Carlo Erba GC 6000, Italy), DB-5 fused silica capillary column (30m x 0.25mm, 0.25 ìm of film thickness). Qualitative analyses were achieved by comparison of mass spectra with those in the NIST library (62000 spectra) and the LIBR (TR) terpene library supplied by Finnigan MAT and those in the literature [3]. The identity of the compounds was confirmed by use of retention indices (RI) measured in this laboratory and obtained from the literature.
Quantitative analysis of components of essential oil was calculated as % of the total oil.
Gas chromatography (GC) with MS detection and flame ionisation detection (FID) showed that the essential oil from leaves of *P. tauricum* contains 27 compounds (above 95% of sesquiterpenes), of which 20 were identified. Predominating compounds in investigated essential oil were: cis-ß-farnesene (30.3-33.5%), caryophyllene oxide (14.2-15.5%), ß-elemene (7.0-7.1%) and ß-bourbonene (3.3-3.8%).

References:

1. Tutin, T.G., Heywood, V.H., Burges, N.A., Valentine, D.H., Walters, S.M., Webb, D.A.: In: Flora Europaea, Cambridge at the University Press, vol. 2 1968.
2. Bartnik M., G³owniak K. and Mardarowicz M.: Acta Poloniae Pharmaceutica – Drug Research, 59, 457-459 (2002).
3. Joulain D. and König W. A.: In: The Atlas of Spectral Data of Sesquiterpene Hydrocarbons, E.B.-Verlag, Hamburg, 1998.

P-09

An overview of vapor-liquid equilibria in the systems containing terpenoids

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The purpose of the present work is to present an overview on vapor-liquid equilibrium (VLE) data for systems containing terpenoids. Terpenoids are rather complicated molecules containing various functional groups.
The literature survey of VLE data, shows the existence of binary and ternary VLE measurements in this attractive field of aroma compounds. So, we found VLE measurements in binary and ternary systems containing: terpenoids and supercritical fluids (carbon dioxide and hydrocarbons) or terpenoids and solvents (ethylic alcohol or/and water) or only terpenoids. The VLE measurements serve for the design of separation processes by distillation in the chemical industry.
We have measured VLE of following mixtures: Methyl chavicole + (1R,4S)-(+)-Fenchone, *trans*-Anethole + (1R,4S)-(+)-Fenchone, Methyl chavicole + *trans*-Anethole, (1S,5S)-(-)-*beta*-Pinene + Eucalyptol, (S)-(+)-Carvone + (R)-(+)-Limonene, Methyl chavicole + Eucalyptol, (R)-(-)-Carvone + Eucalyptol, Methyl chavicole + *trans*-Anethole + (+)-Fenchone, Octane + (+)-Limonene, (R)-(-)-Carvone + Decane, (-)-Menthone + Decane and (1R,4S)-(+)-Fenchone + Decane.
Our VLE measurements were planned to meet two requirements: first, accurate vapor-liquid equilibrium data are necessary for the design of separation processes (batch distillation) and second, to check the applicability of group contribution models (DISQUAC and UNIFAC) to predict the VLE data in mixtures containig terpenoids. In order to investigate the intramolecular efects of polar groups and double bonds on the group interaction parameters of the mentioned models it was necessary to examine first mixtures of terpenes with a relatively inert solvent such as an alkane.

The DISQUAc model, using the dispersive and quasichemical parameters, taken from previous publications, is appropriate for the investigated terpenoids, except. the binary system n-decane + (+)-fenchone where the strong steric effect hindrance of the methyl groups on carbonyl group affects the quality of prediction. The UNIFAC group-contribution model predictions are satisfactory in most cases except in systems containing (-)-carvone or (+)-fenchone where the agreement is rather poor.

References

1. I. Wichterle, J. Linek, Z. Wagner and H.V. Kehiaian Vapor-Liquid Equilibrium in Mixtures and Solutions. Bibliographic Database. EVLM'2000 CD-ROM ISBN 2-9507664-2-0 Publisher ELDATA 6, Rue Lacepede, 75005 Paris FRANCE
2. I. Batiu, ELDATA: Int. Electron. J. Phys.-Chem. Data 5 (1999) 1-5.
3. I. Batiu, ELDATA: Int. Electron. J. Phys.-Chem. Data 5 (1999) 191-195.
4. I. Batiu, Fluid Phase Equilibria 198 (2002) 111-121

P-10

Chemical composition of the essencial oils of *Minthostachys setosa* (Briq.) Epl. (Lamiaceae) from Perú

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Minthostachys setosa (Briq.) Epl. is an aromatic shrub, distributed in the south of Perú: especial around of Cuzco town (Valle de Paucartambo, Pillahuata), Puno (Sicuani, Meseta del Callao) Ayacucho and Apurimac. It was described for the first time in the XVII century like a similar plant of oregano, but with the smaller leaves and the clean green color. The fragrances white flowers are similar to cabbage but smaller. The leaves and flowers spikes are used as a spice in foods. The native Indians use the plant in folk medicine to cure the tumour and leaves in mixture with *chilca*, in bone fracture. The essential oils of *Minthostachys setosa* is used as pesticide, for the food conservation (against *Phytphtora intestinats, Fusarium solanaceum* and *Erwinea corotovora*), insecticide (against *Musca domestica*) and bacteriology (against *Shigela dysenteriae, Salmonela typhi* and *Eserichia colli)*. Also the essential oil has anti-inflammatory, carminative, antiseptic and analgesic action.

Therefore, in view of its local importance in traditional medicine, the present study was undertaken in order to increase knowledge of the chemical composition of the essential oils of *Minthostachys setosa* aerial plant from the south of Perú.

Aerial parts of *Minthostachys setosa* were collected at full flowering stage, in the areas of Ayacucho, the south of Perú. The essential oil was isolated by dydrodistillation for 30 min. The essential oil was limpid, with a pleasant mint odour. The content of volatile oil was 3.0% (v/w) on dry weight basis.

GC analyses were carried out with a Hewlett-Packard 6890 gas-chromathograph equipped with a flame ionization detector. The sample was analyzed on two fused silica capillary columns with bonded phases of different polarity.

The identity of the components was assigned by comparison of their RIs, relative to C9-C23 n-alkanes, with those of authentic standards available in our own laboratory or with GC data previously published [4].

GC-MS analyses were performed on a Hewlett-Packard 5890 series II gas-chromatograph coupled with a Hewlett-Packard 5989 B mass-spectrometer. Compounds were identified using both chromatographic and mass spectroscopic criteria.

Identites of compounds were established by use of on-line Willey275/ NBS75k/ NIST mass spectral data bases and literature MS data [5].

References

1. F. Senatore, *Flavour Fragr. J.* **13**, 263-265 (1998)
2. N.W.Davis, *J. Chromatogr.* **503,** 1-24 (1990)
3. Y. Masada, *Analysis of Essential Oils by Gas Chromatography and Mass Spectrometry,* John Wiley & Sons, New York, 12-19 (1976)

P-11

Antifungal activity of the essential oil of *Ziziphora clinopoides* Lam from Iran

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Antifungal acitivities of different concentrations of the essential oil of *Ziziphora clinopoides* Lam, was evaluated against four filamentous fungi and one yeast strain. The antifungal tests were conducted by a Poisoned food technique against the filamentous fungi (*Aspergillus niger*, *Trichophyton rubrum*, *Trichoderma reesei* and *Microsporum gypseum*) and, by a microdilution assay against *Candida albicans*.
The essential oil was obtained from the leaves of *Z. clinopoides*., by a Clevenger apparatus (1). The minimum inhibitory concentrations (MICs) of the oil against the filamentous fungi were determined according to Grover and Moore (2). The requisite quantity of the oil samples were mixed in acetone (2% of the required quantity of the medium) and then added in pre-sterilized SDA medium, pH 5.6. Mycelial discs of 5 mm diameter cut out from the periphery of seven day old cultures were aseptically inoculated upside down on the agar surface of the medium. Inoculated Petri plates were incubated at 27 ± 1°C and the observation recorded on the seventh day. The MIC against *C. albicans* was determined by a microdilution assay (3). The oil was found to be fungicide against *Trichophyton rubrum* at $1\mu l.ml^{-1}$ (1000 ppm). The MIC_{100} of oil against *Trichoderma reesei* and *Microsporum gypseum* was found to be $0.5\mu l.ml^{-1}$ while this concentration of the oil exhibited % 58.2 mycelial growth inhibition for *A. niger*. Also an MIC of $1\mu l.ml^{-1}$ (1000 ppm) was obtained for the oil against *C. albicans*. It could be concluded from the present study that there seemed to be a direct correlation between the oil concentration and bioactivity against the test organisms and that different fungi exhibit different susceptibility profiles to *Z. clinopoides* essential oil.

References:

1. Clevenger, J. F. (1928) *J. Am. Pharm. Assoc.* **17**, 346.
2. Grover, R. K., Moore, J. D. (1962) *Phytopathol.* **52**, 876-880.
3. Ellof, J. N. (1998) *Planta Medica* **64**, 711-713.

P-12

Seasonal Variation of the Essential Oil Composition of Labrador Tea (*Ledum groenlandicum*)

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The sweet, spicy aroma leaves of bog Labrador tea, can be used to make a palatable tea. As a folk medicine, the tea was used externally for all kinds of skin problems. Taken internally, the tea was used to stimulate the nerves and stomach. Syrups made from the tea were sometimes used for coughs and hoarseness.
Labrador tea (a name reflecting the northern distribution and the common use as tea by native North Americans), is also named common Labrador tea, bog Labrador tea, bog tea, Hudson's Bay tea, James tea, St. James tea, Indian tea or wooly tea.
Labrador tea is a low, native, evergreen shrub from 0.3 to 1.2 m high distributed throughout Alaska, Canada and Greenland. It occurs south through New England, the northern parts of the Lake States, northern Idaho, and western Washington and Oregon. The leaves are 2.5-7.5 cm long, leathery in appearance, conspicuously rolled under at the margins, and densely wooly underneath, this fuzz becoming a deep rust colour as the leaves mature. Glandular hairs, especially on the leaves and younger branches, synthesize essential oil responsible for the aroma and medicinal qualities of the plants.
Labrador tea (Ledum groenlandicum) have been harvested from Grondines in Mauricie Region (Quebec) at three different times during the growing season. The essential oils of the aerial part of the plants were isolated by steam distillation of fresh plant and 24 hours dry plants. The essential oil were analysed by capillary gas chromatography (GC). Compounds were identified by their mass-spectra and retention indices (Kovat's) relatives to n-alkanes on polar and apolar capillary column. The main component found in the young leave is β-phellandrene and germacrone is the main component of old leaves. Sabinene was much higher in young than in old leaves; Myrcene and Cineol were found just in young leaves and Germacrone and α-Terpinene were found just in old leaves. The best yield in essential oil is obtained in june and β-phellandrene is dominant at near 70% and decrease to 35% in July to fall at 10% in August.

References:

Carleton, T. J.; Maycock, P. F. 1980. Vegetation of the boreal forests south of James Bay: non-centered component analysis of the vascular flora. Ecology. 61(5): 1199-1212.

Reichardt, P. B.; Bryant, J. P.; Anderson, B. J.; [and others]. 1990. Germacrone defends Labrador tea from browsing by snowshoe hares. Journal of Chemical Ecology. 16(6): 1961-1970.

P-13

Fresh Saffron stigmas to typical dried spice: Evolution of organoleptic properties

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Saffron is a high-value spice obtained from dried *Crocus sativus Linn.* stigmas. It is widely used as a condiment for its delicate flavour and intense orange-red colour. Dye properties are caused by crocin, a C_{20}-carotenoid gentiobiose diester. The major constituent of saffron's volatile fraction, safranal, is formed by hydrolysis of the bitter glycoside picrocrocin. The freshly picked stigmas give not the typical saffron flavour which is developed during the drying process.

Our specific objective consisted in determining the influence of the drying process on the quality of the spice. Eleven samples of fresh stigmas, from Quercy area (France) and from six different harvests, were used for these studies and both dried by producers and in laboratory. Fresh stigmas odour have been analysed by DHS/GC-MS and compare to the corresponding aromatic profiles of dried stigmas. The organoleptic quality of saffron samples, was first evaluated at different moisture values using DHS and SPME/GC-MS. Simultaneously, the quantitative determination of secondary metabolites, crocin, picrocrocin and safranal was performed by UV spectrophotometry. Different characteristic fingerprints have been observed on aromatic profiles. Variation of moisture values showed a big impact on the quantity of crocin and consequently on the quality of the spice.

P-14

Characterisation of oregano (Origanum vulgare L.) lines of high quality

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Oregano can be considered as one of the most important Mediterranean spices, which shows rather high diversity from both taxonomical and chemical point of view (Bernáth, 1997). The importance of oregano is increasing continuously. Beyond its flavouring properties antimicrobial, antiviral, nematicidal and antioxidant activities of the plant drug and its essential oil have been proved.

In open field experiments individuals of 12 selected lines of *Oiganum vulgare* L. and 5 lines of *O. vulgare* L. subsp. *hirtum* Ietswaart (*O. heracleoticum* sensu) were investigated and compared. Morpho-phenological, production biological and essential oil accumulation properties of the individuals were measured and evaluated. To identify essential oil content the samples were distilled in Clevenger apparatus. The composition of the oil was analysed by GC method (Shimadzu GC-B14 with a FID detector and a Shimadzu C-R5A Chromatopac integrator).

In harmony with literature references the essential oil content of individuals belonging to the O. *vulgare* lines was rather law, ranging about 0,07-0,33 %. In contrast the essential oil content measured in the individuals of the *O. vulgare* subsp. *hirtum* were much higher, reaching 7 per cent in some lines. Taking into consideration the compositional characteristics of all *O. vulgare* subsp. *hirtum* lines belong to the "carvacrol group" described by Pasquier (1997). However, according to our results the individuals may classify into four subgroups, which are as follows:

a) high carvacrol, b) middle carvacrol – middle γ-terpinene – middle p-cymen, c) low carvacrol – high γ-terpinene, d) low carvacrol – high γ-terpinene – high p-cymen.

Bernáth, J. 1997. Some scientific and practical aspects of production and utilisation of oregano in Central Europe. Oregano. Proceedings of IPGRI Workshop (8-12 May 1996) Bari, Italy 76-93.

Pasquier, B. 1997, Selection work on Origanum vulgare in France. Oregano. Proceedings of IPGRI Workshop (8-12 May 1996) Bari, Italy 94-102.

P-15

Essential oil of wild *Hypericum perforatum* L. from Eastern Lithuania

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The chemical composition of the essential oils of *Hypericum perforatum* L. growing wild in ten habitats in Eastern Lithuania was studied. The aerial parts of plants were collected in 2001 at full flowering and air dried at room temperature (20 – 25^{0}C). The essential oils (0.1 – 0.4 %) were prepared by hydrodistillation of 10 – 100g air dried samples. The analyses of the essential oils were carried out by GC and GC – MS. HP 5890 II chromatograph equipped with FID and a capillary column HP – FFAP was used for quantitative analyses. Analyses by GC – MS was performed by chromatograph 5980 II interfaced to a HP 5971 mass spectrometer and equipped with capillary column CP – Sil 8 CB. The percentage composition of the essential oils was computed from GC peak areas without correction factors. Qualitative analyses was based on the comparison of retention indexes and mass spectra with corresponding data in the literature and the computer mass spectra libraries (Wiley and NBS 54K).

Forty six identified constituents made up 85.3 – 97.2 % of the essential oils. Four essential oils under study were of β-caryophyllene (10.5 – 19.1 %), four samples – of β-caryophyllene oxide (13.3 – 35.8 %) and two oils – of germacrene D (16.1 – 31.5 %) chemotype according to the first major constituent. The quantities of spathulenol in the oils of β-caryophyllene and caryophyllene oxide chemotypes were 5.4 – 8.5 %. The above compound was between four main constituents. The essential oils were rich in sesquiterpenoids (62.0 – 81.8 %). The amounts of compounds with caryophyllane skeleton made up 17.3 - 46.9 %. Identified aliphatic compounds varied from 1.7 to 19.6 %. Germacrene D was not detected earlier as the first major constituent in *Hypericum perforatum* species.

P-16

Essential Oils of *Phlomis caucasica* Rech. f. and *Phlomis olivieri* Benth. from Iran

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The genus Phlomis is comprised of about 100 species, seventeen are describe in the flora of Iran, among which ten are endemic.
The water distilled essential oils from aerial parts of *Phlomis caucasica* and *Phlomis oliveri*, which are endemic to Iran, were analyzed by GC and GC/MS.
The oil of *P. caucasica* was found to contain alpha-pinene (82.2).
The oil of *P. oliveri* was characterized by higher amount of germacrene D (26.4%) and bicyclogermacrene (12.7%).

P-17

Some Problems with GC Analysis of Essential Oils in the Pharmacopoeias

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Department of analytical chemistry of the State Institute for Drug Control together with Faculty of Pharmacy attempted to improve methods for analyses of essential oils. That improvement we realized in the last five years in the form of diploma and post-gradual works in six stages:

1. Development of methods easy reproducible in the most laboratories.
   - We tried to replace conventional capillary columns (ID = 0.25 - 0.32 mm) by megabore capillary ones (ID = 0.53 mm) both polar (DB-WAX) and very low polar (DB-5).
2. Development of the fast method.
   - We studied in details "Fast GC" methods performed on the polar and non-polar columns 10 m long, with inner diameter 0,10 mm. We achieved approximately 5 to 10 times shorter time of analyses.
3. Attempt to simplify identification of components without using large number of standards.
   - We confirm very large applicability of the comparison linear retention indexes of the components with tabulated dates. This method is useful not only for individual essential oils but also for very rich mixtures analysed on many columns of different dimensions.
4. Unification of the temperature programs of pharmacopoeial methods of analyses of essential oils.
   - We confirm possibility to analyse almost all essential oils under the same conditions. This fact also very simplifies identification of components in essential oils.
5. Attempt to achieve good and unambiguous reproducibility of pharmacopoeial methods.
   - We revealed some mistakes in European pharmacopoeias during the control of all gas chromatographic methods of essential oils analyses.
6. Innovation of some "old-fashioned" methods published in national articles of Czech Pharmacopoeia 1997 in connection with issuing new Czech Pharmacopoeia 2002.

P-18

On the Antimicrobial Activity of Sandalwood Essential Oils

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In continuation of our studies in sandalwood chemistry as well as regarding the bioactivity of Essential Oils (EO) and fragrance compounds, it seemed worthwhile to compare sandalwood oils of different origin and even from another plant family but belonging to the same odor class, as to their antimicrobial activities. Three charges of Australian sandalwood oil (*Santalum spicatum*, Santalaceae) - an extract and two steam distillates -, then a sample of East Indian sandalwood oil (*Santalum album*, Santalaceae), further a commercially available sample of a mixture of α- and β-santalol, and finally a sample of the previously referred West Indian sandalwood oil (*Amyris balsamifera*, Rutaceae), now correctly known as amyris oil, were tested for their bioactivity against some gram-(+)- and gram-(-)-bacteria and the yeast *Candida albicans*.

As a result we found: 1) The steam distillate of Australian sandalwood oil with a high content of sesquiterpenoid alcohols (>96%, comprising α- and β-santalol, trans-nuciferol, trans,trans-farnesol, α-bergamotol and α-bisabolol) only showed a bacteriostatic effect against the two gram-(-)-bacteria strains *Escherichia coli* and *Klebsiella pneumoniae*, but no bacteriostasis against the other microorganisms. 2) In that way, the effect of the commercially available santalol mixture resembled the afore mentioned sample of *S. spicatum* with the addition that also a strong inhibition of the growth of *Staphylococcus aureus* could be observed. 3) The extract of Australian sandalwood oil (lower concentration of *E*-nerolidol, β-bisabolol, α-bisabolol and *trans,trans*-farnesol within a similar total sesquiterpenoid alcohol mixture as before), East Indian sandalwood oil as well as a complete steam distilled EO of *S. spicatum* inhibited the growth of all test microorganisms. The best effect was observed against *S. aureus* after administration of the Australian sandalwood extract. A lesser activity showed East Indian sandalwood oil, and even no effect against *Pseudomonas aeruginosa*, *Bacillus cereus* and *Candida albicans*. 4) Finally, West Indian sandalwood oil showed a different behavior and was effective only against *S. aureus* and to a lesser extent against *P. aeruginosa*.

P-19

Biogenetic Studies in *Syringa vulgaris* L.: Bioconversion of $^{18}O(^{2}H)$-Labeled Precursors into Lilac Aldehydes and Lilac Alcohols

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The novel plastidic DOXP/MEP pathway has been described as the dominant route for monoterpene biosynthesis of lilac aldehyde and lilac alcohol in lilac inflorescences.
Feeding experiments with ^{18}O-labeled linalool were carried out, in order to clarify the cyclization mechanism to lilac aldehyde stereoisomers.
Furthermore the location of *de novo* biosynthesis inside the cells of flower petals is studied in more detail. For that reason the chloroplasts were isolated. Flower petals, which either were detached from inflorescences after feeding with suitable precursors or first detached from inflorescenses and subsequently incubated with solutions of suitable precursors were investigated.
Moreover, feeding experiments with isolated chloroplasts were carried out.
The volatiles of isolated chloroplasts were analysed by stir bar sorptive extraction (SBSE) and enantioselective multidimensional gas chromatography (enantio-MDGC/MS) allowing the simultaneous detection of genuine and labeled monoterpenoids.

References

[1] Kreck, M., Püschel, S., Wüst, M., Mosandl, A. (2003) *J. Agric. Food. Chem.* **51**, 463-469
[2] Kreck, M., Mosandl, A. (2003) *J. Agric. Food Chem.* **51**, 2722-2726
[3] Burkhardt, D., Mosandl, A. (2003) *J. Agric. Food Chem.* (in press)

P-20

Glycosidic Conjugates of Monoterpene Alcohols, Cucurbates and C-13 Norisoprenoids in *Boronia megastigma*

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Enzymatic hydrolysis of a glycosidic fraction of boronia marc, obtained using XAD2 chromatography, yielded a complex mixture of monoterpene, C-13 norisoprenoid and cucurbate volatiles. Results obtained using β-D-glucosidase and the pectinase, AR2000, were compared and considered with regard to the disappearance of proposed glycoside and malonyl glycoside conjugates detected by APCI LC-MS. Liberated volatiles were measured using GC-FID and identified by GC-MS by comparison with known spectra and retention times. Major volatiles released during enzymic incubation included linalool, 8-hydroxy-linalool, 2,6-dimethylocta-3,7-dien-2,6-diol, 3-hydroxy-5,6-dihydro-β-ionone, 3-hydroxy-β-ionone, 4-hydroxy-β-ionone, methyl cucurbate, methyl epicucurbate and methyl diepicucurbate.

P-21

Composition of the essential oil from the fruits of *Schinus molle* L. (Anacardiaceae) from Peru

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Schinus molle L.(common names: Peruvian peppertree, molle del Peru) is a shrubby tree with narrow, spiky leaves, which grows 4 to 12 m tall. It is indigenous to South and Central America, and can be found in semitropical and tropical regions. Its reddish fruits have been used, among with those of other *Schinus* species, as a substitute of pepper. Therefore these species are also called peppertrees.

The Peruvian peppertree grows in the valleys and slopes of the Andes Mountains, at altitudes up to 3300 m above sea level in the Southern Andes, up to 3000 m in the Central Andes and up to 2000 m in the northern regions.

The plant has been used medicinally by indigenous people throughout the tropics for very long time. In Peru, the sap is used as a purgative and diuretic, and the entire plant is used externally for fractures and as a topical antiseptic. The oleoresin is used externally as a cicatrizant of wounds and for toothaches, and it is taken internally for rheumatism, a folk disease called *suto* and as a purgative. The berries, which have a peppery flavor, are used in Peru in syrups, vinegar and beverages.

All parts of the tree are rich in essential oil, that produce a spicy, aromatic scent. The fruits can contain up to 5% essential oil, and the leaves can contain up to 2% essential oil.

The plant material investigated in this study were the fruits of *Schinus molle* L, harvested ashore of the Chillón river, near Lima, in September 2002. The essential oils were obtained by hydrodistillation of the dried, crushed fruits, using a Clevenger type apparatus. The oil yield varied from 3,5 to 3,9% (mass/dry weight).

The oils were analyzed by GC and coupled GC-MS, by dual channel analysis using two 60m fused silica capillary columns with stationary phases of different polarity (SPB-1 and Supelcowax-10) . Identification of the compounds was performed using MS library search in combination with retention indices.

The main components, representing up to 94% of the total oil were: α-pinene (3,1÷5,7%), myrcene (26,4÷42,0%), α-phellandrene (4,0÷25,0%), limonene (9,8÷19,0%), β-phellandrene (7,7÷9,7%), p-cymene (3,2÷19,8%), methyl octanoate (0,7÷1,9%), β-caryophyllene (0,5÷0,9%).

The enantiomeric distribution of the main chiral monoterpene hydrocarbons was determined by GC separation using a 30 m fused silica capillary column coated with modified cyclodextrins as the stationary phase (β-Dex 325). The ratios were found to be as follows:
(1R,5R)-(+)-α-pinene (92,6÷96,5%) : (1S,5S)-(–)-α-pinene (3,5÷7,4%)
(5S)-(+)-α-phellandrene(100%): (5R)-(–)-α-phellandrene(0%)
(4R)-(+)-limonene(20,2÷20,5%): (4S)-(–)-limonene(79,5÷79,8%)
(6S)-(+)-β-phellandrene(100%): (6R)-(–)-β-phellandrene(0%).

Taylor, L. (1998) *Herbal Secrets of the Rainforest*, Prima Publishing, Rocklin, CA
Rossini, C., Menendez, P., Dellacassa, E., Moyna, P. (1996) *J.Essent. Oil Res.* **8**, 71-73
Adams, R. (1995) *Identification of Essential Oil Components by Gas Chromatography/Mass Spectroscopy*, Allured Publ..Co., Carol Stream, Illinois, USA.

P-22

Chemical and Biological Investigations of *Salvia* Essential Oils

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Lamiaceae comprise a variety of aromatic plants with about thousand different *Salvia* species. *Salvia hedgeana* Dönmez (new species), *S. huberi* Hedge, *S. pisidica* Benth. growing in Turkey were collected and subjected to hydrodistillation. The essential oils of aerial parts yielded were analyzed both by gas chromatography – flame ionization detection (GC-FID) and gas chromatography – mass spectrometry (GC-MS). *S. hedgeana* essential oil consisted of ß-pinene (30.0%) as major component among 65 identified components representing 89.9% of the total oil. The major component of *S. huberi* was identified as 1,8-cineol (20.4%), and 76 further components were characterized representing 87.6%. *S. pisidica* essential oil revealed the occurrence of camphor (21.7%) as the main constituent among other 59 identified components of 76.8% of the total components. The biological activity of the essential oils was tested on the chorioallantoic membrane (CAM) of the fertilized hens` egg in order to examine the anti-angiogenic and anti-inflammatory activity as well as irritant or toxic effects, where the CAM assay is applied as a successful *in vivo* method. The essential oils at a concentration of 125 µg/pellet, showed no anti-inflammatory, –angiogenic or toxic effects.

P-23

Solid-Phase Microextraction and Headspace Sorptive Extraction of the Volatile Fungal Metabolites Produced by Toxigenic *Fusarium* Species

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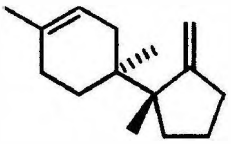
Fungal infection in stored foods and cereals decreases their nutritional value and can pose health hazards because of the formation of mycotoxins. There is thus a need for methods that can accurately quantify the degree of fungal infection in grains at an early stage of mould growth. An efficient methodology was developed to determine the growth of toxigenic *Fusarium*, based on the headspace solid-phase microextraction and stir bar sorptive extraction in the headspace mode (HSSE) of the fungal volatile metabolites produced.
Fungi are known to produce a wide range of volatile secondary metabolites, many of which belong to the class of hydrocarbon sesquiterpenes [1]. One of these fungal sesquiterpenes is trichodiene, an intermediate in the biosynthesis of trichothecenes, produced by *Fusarium* sp.



Trichodiene

Previously we reported the use of solid phase microextraction and stir bar sorptive extraction as monitoring technique for the collection and detection of the fungal volatile metabolite (+)-aristolochene by sporulated surface cultures of toxigenic strains of *Penicillium roqueforti* [2,3]. This paper describes the use of SPME and HSSE (headspace sorptive extraction) for the fast detection of trichothecene producing *Fusarium* spp. This method is based on the monitoring of the *de novo* production of trichodiene. Different growth conditions and media, such as malt extract agar and potato dextrose agar were compared. It was found that trichodiene was only produced by toxigenic strains of *Fusarium sambucinum* and *F. sporotrichioides*. It was the main volatile metabolite in the headspace extract of the cultures. Non toxigenic *Fusarium* strains, on the other hand, showed a remarkably different headspace profile.

[1] T.O. Larsen, J.C. Frisvad, *Mycol. Res.* 99 (1995) 1153.
[2] J.C.R. Demyttenaere, A. Adams, K. Van Belleghem, N. De Kimpe, W.A. König, A.V. Tkachev, *Phytochemistry* 59 (2002) 597.
[3] J.C.R. Demyttenaere, R.M. Moriña, P. Sandra, *J. Chromatogr.* A 985 (2003) 127.

P-24

Comparison of Steam Distillation Solvent Extraction with Solid Phase Microextraction and Headspace Sorptive Extraction for the Analysis of the Key Fragrance Compounds of *Wisteria sinensis*

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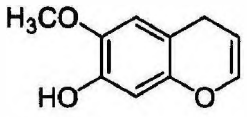
Recently, a number of volatile compounds have been isolated from the flowers of *Wisteria sinensis*, a popular garden plant (Leguminosae), which blooms in May with large clusters of violet flowers [1]. 6-Methoxy-4*H*-1-benzopyran-7-ol **1** was isolated from the hexane extract of the flowers as a key flavour compound, imparting the characteristic smoked odour to this flower, along with 6,7-dimethoxy-*4H*-1-benzopyran **2** [1].
Three sample preparation techniques were compared for the GCMS analysis of blossoms of *Wisteria sinensis*, namely steam distillation solvent extraction, solid phase microextraction (SPME) and headspace sorptive extraction (HSSE).
Therefore freshly picked blossoms of *Wisteria sinensis* were steam distilled with CH_2Cl_2 as extraction solvent using a Likens-Nickerson extraction device. The dried extract was analyzed by GCMS and contained 2.6% of 6-methoxy-4 *H*-1-benzopyran-7-ol **1** and 11.0% of 6,7-dimethoxy-*4H*-1-benzopyran **2**.



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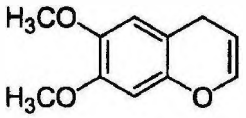

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Some blossoms were also sampled by headspace solid phase microextraction, using polydimethylsiloxane (100 μm) as the stationary phase. In the headspace SPME extract of the flowers only one of the character donating compounds of the flowers was detected, namely 6,7-dimethoxy-*4H*-1-benzopyran **2** contributing to 2.9% of the total volatiles.
Comparable results were obtained when the flowers were sampled by the novel extraction technique, stir bar sorptive extraction (SBSE) in the headspace mode, *i.e.* headspace sorptive extraction (HSSE).
Compounds **1** and **2** were identified by mass spectrometry, and the exact structure of 6-methoxy-4*H*-1-benzopyran-7-ol **1** was confirmed by organic synthesis through elaboration of 7-hydroxy-6-methoxycoumarin (scopoletin) [2].

[1] D. Joulain, R. Tabacchi, Phytochemistry 37 (1994) 1769.
[2] J. Demyttenaere, K. Van Syngel, A.P. Markusse, S. Vervisch, S. Debenedetti, N. De Kimpe, Tetrahedron 58 (2002) 2163.

P-25

Essential Oil Composition of Different Distilled Fractions of *Artemisia dracunculus* L. from Mongolia

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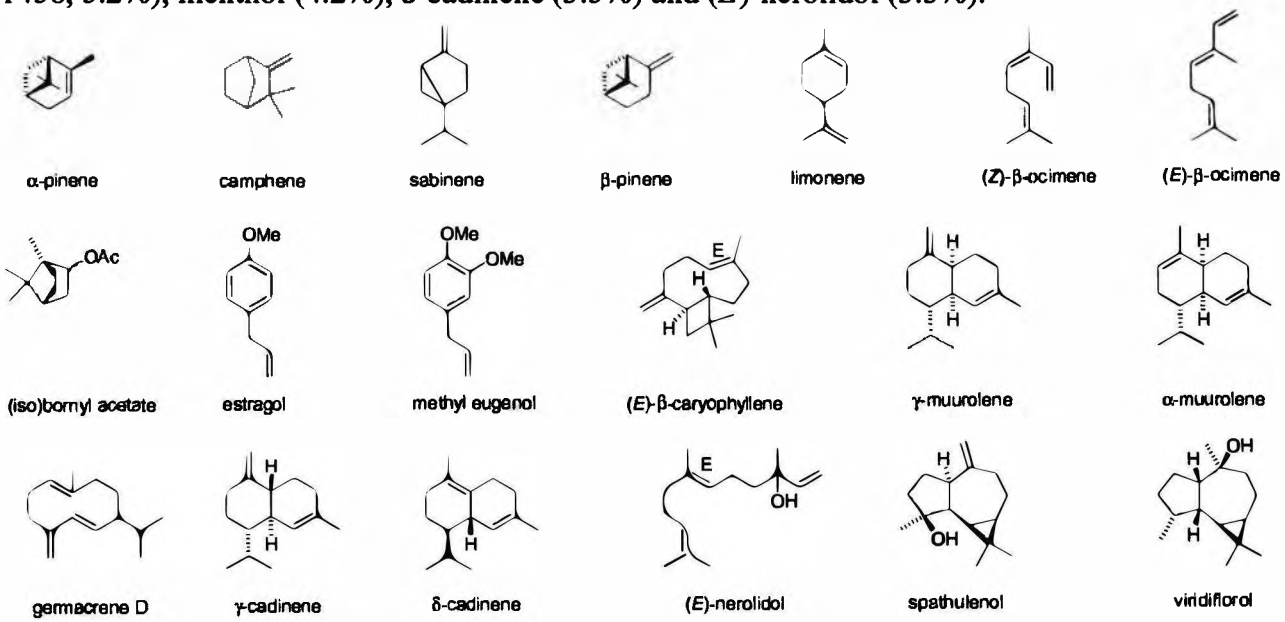
The essential oil composition of *Artemisia dracunculus* L., growing in Mongolia, was investigated using combined vacuum distillation techniques and gas chromatography-mass spectrometry.

Samples of the aereal parts of this plant were collected in the region of the Bogd mountains, Mongolia. The essential oil, obtained by steam distillation (yield 1.27%), was first analysed by GC-MS and was then separated by vacuum distillation in three fractions. One fraction (4.3 ml) was obtained during distillation at 147-178 °C, the second fraction (3.2 ml) was collected during distillation at 227-267 °C, and the third fraction (2.5 ml) was the remaining non distilled fraction. All fractions were dissolved in hexane for separate analysis by GC-MS.

It was found that the crude essential oil before separating into three fractions contained mainly sabinene (31.5%), methyl eugenol (10.6%), (*E*)-nerolidol (9.4%), (*E*)-β-ocimene (9.1%), (*Z*)-β-ocimene (8.1%), β-pinene (7.1%), estragol (4.9%) and β-myrcene (4.1%).

The first fraction obtained during distillation between 147 and 178 °C contained only monoterpene hydrocarbons with as main constituents α-pinene (54.1%), limonene (14.4%) and camphene (8.1%). The second fraction recovered during distillation between 227 and 267 °C was the most complex and rich fraction, composed of monoterpenoids and sesquiterpenoids. Main volatiles were (iso)bornyl acetate (31.9%), γ-cadinene (7.8%), α-muurolene (5.6%), (*E*)-caryophyllene (4.4%), γ-muurolene (2.6%), spathulenol (2.5%) and δ-cadinene (2.4%).

The main constituents of the remainder (non distilled fraction) were viridiflorol (30.0%), germacrene D (14.5%), three unidentified terpenes (RI 1295, 7.6%, RI 1497, 7.3% and RI 1458, 5.2%), menthol (4.2%), δ-cadinene (3.5%) and (*E*)-nerolidol (3.3%).



P-26

Characterisation of Oxygen Heterocyclic Components of Cold-pressed Citrus Essential Oils

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The oxygen heterocyclic compounds (coumarins, psoralens and polymethoxylated flavones (PMFs)) present in citrus essential oils (lemon, mandarin, sweet orange, bitter orange, bergamot, grapefruit and lime) were analysed by reversed phase HPLC using both conventional and monolithic columns. UV and MS spectra were obtained using photodiode array and mass spectrometer (API/MS system equipped with an APcI source in positive mode) detectors.

MS spectra were recorded at different voltages to obtain structural information in addition to molecular weight information. The different response of the three classes of compounds was evaluated, and conditions suitable for the contemporary ionisation of all the components were optimised. UV and MS spectra were used for the identification of the components in the citrus oils.

Monolithic column could operate at higher flow-rate than a conventional RP column with a reduced pressure drop and shorter washing and re-equilibration times. This produces a faster separation of oxygen heterocyclic compounds. Because of their better mass transfer properties, these columns maintain high separation efficiency, even at high linear flow rates. The possibility of analysing many samples in a very short period of time and obtaining the same information than with conventional columns can allow laboratories to make considerable time savings.

This method allowed the rapid identification and the characterisation of the oxygen heterocyclic compounds of citrus oils, the detection of some minor components for the first time in some oils, and the detection of authenticity and possible adulteration of the oils.

P-27

Simultaneous Distillation-Extraction of Water-Soluble Constituents of Rose Oil

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Simultaneous distillation-extraction (SDE) has been one of the most often cited methods for the isolation of volatiles since its first report by Likens and Nickerson in 1964. In recent years, a special design of this apparatus has been fabricated which permits consideration of the preparative isolation of volatiles on a laboratory scale for subsequent fractionation and analysis, as well as industrial scale operations. As an interesting field of research, extraction of water-soluble aroma constituents of rose oil from rose water and second distillation water using the SDE may be considered. In this study, preliminary experiments were carried out to study the efficiency of the process. Extractions were conducted on binary test mixtures of water and 2-phenylethanol using different solvents such as n-butyl acetate, n-hexane and iso-butanol. Concentrations of 2-phenylethanol in the extracts were determined by GC analysis. Concentrations in raffinate phases were determined by UV measurement in at 257.5 nm. The results of the experiments as well as the best condition for the extraction of 2-phenyl ethanol are presented.

References

1. Pollien, P. and Chaintreau A. *Anal. Chem.* 1997, **69:** 16, 3285-3292.
2. Pollien, P., Ott, A., Fay, L.B., Maignial, L., Chaintreau, A. *Flavour and Fragr. J.* 1998, **13:** 413-423.
3. Chaintreau, A. *Flavour and Fragr. J.* 2001, **16:** 136-148.

P-28

Phytochemical and Biological studies of Moroccan *Carum carvi*

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The fruits of carvi or *Carum carvi*, are used in Moroccan popular medicine in the case of flatulence, indigestion and colic. This plant which belongs to the family of the Umbelliferae is cultivated in various regions in our country and its fruits are exploited currently in the preparation of the bread. An earlier phytochemical study on *Carum carvi* focused on the main components of the essential oil and led to the isolation of carvone and limonene with a high purity respectively with 97 and 95 %. The qualitative and quantitative oil analysis were realized by GC and GC/MS. Thirthy-five compounds representing over 91 % of the oil were identified.

The aim of this study was to investigate the different extract prepared from the fruits in order to improve the knowledge about its phytochemical composition and to identify compounds responsible of the activity. Both the ethanolic, methanolic and hexanic extracts prepared from dry fruits were checked for their antimicrobial (against Gram-positive and Gram-negative bacteria) and antioxidant activities. The ethanolic extracts showed remarkable antioxidant activity.

The differents extracts obtained showed the presence of coumarins, flavonoids and triterpenes. They were subjected to column chromatography. The organic constituents will be separated by TLC, HPLC and the structures will be deduced from spectroscopic analysis (IR, UV, ^{1}H-NMR) and mass spectrometry.

P-29

Antibacterial activity of the essential oil of *Cymbopogon schoenanthus* ssp. *proximus*

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In previous studies on the chemistry of the essential oil of *Cymbopogon schoenanthus* ssp. Proximus [1] and [2], it was reported that the aerial part oils are composed mainly of piperitone, elemol, (+)-2-carene, beta-eudesmol, gamma-eudesmol and limonene. In this work we report on the antibacterial activity, by well diffusion technique on Muller-Hinton agar, of the hydrodistilled essential oil isolated from aerial part samples of *C. schoenanthus* ssp. Proximus, collected during dry season from Jebel Arffal , Ed-Damer region (around 17° 34 N latitude and 33° 56 E longitude) north central Sudan. The findings revealed that *C. schoenanthus* ssp. Proximus essential oil remarkably inhibited the growth of tested clinical isolates Gram- positive (*Staphylococcus aureus* , *Bacillus subtilis*) and Gram-negative (*Escherichia coli*, *Proteus vulgaris*) bacteria except for Gram-negative, *Pseudomonas aeruginosa*. Reference antibiotic disks such as Ampicillin, Tetracycline, Chloramphenicol, Gentamicin, Ofloxacin and Ciprofloxain were used for comparison. Further studies on other bacteria and some pathogenic fungi, would be interesting.

[1] Banthorpe D., Duprey R., Hassan M., Jones J., Modawi B., Planta med., 29, 10-18, 1976.

[2] EL-Kamali H.H., Khalid H.E., Fadlalla B., Hassan M.H., EL-Kamali H.H., 33nd International Symposium on Essential Oils, Lisboa, Portugal,. Abstract Book :104 , Sept. 2002.

P-30

Volatile Constituents of *Centaurea depressa* M.B. and *Carduus pycnocephalus* L., Two Compositae Herbs Growing Wild in Iran

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The essential oils from two Compositae species of Iran: *Centaurea depressa* M.B and *Carduus pycnocephalus* L. obtained by hydrodistillation were analyzed by GC and GC/MS.
The oil of *Centaurea depressa* consisted of four oxygenated monoterpenes (36.5%), six sesquiterpene hydrocarbons (5.9%), ten oxygenated sesquiterpenes (39.7%), five aliphatic hydrocarbons (4.4%) and one aliphatic acid (4.0%). Piperitone (35.2%) and elemol (14.1%) were the major components in this oil, followed by β-eudesmol (6.9%), spathulenol (5.0%), caryophyllene oxide (4.0%) and hexadecanoic acid (4.0%).
The oil of *Carduus pycnocephalus* consisted of five sesquiterpenes (8.5%), fourteen benzene derivatives (33.2%), three aliphatic acids (28.6%), five aliphatic hydrocarbons (2.7%), one aliphatic ketone (7.4%) and one C_{13}-compound (1.0%).
The major component of this oil was hexadecanoic acid (23.3%) followed by dibutyl 1,1,2-benzene dicarboxylate (8.2%), 6,10,14-trimethyl 2-pentadecanone (7.4%) and tetradecanoic acid (4.3%).
The aerial part of two Compositae species were collected at the following place: 150 g of C*entaurea depressa* and 200g of *Carduus pycnocephalus* collected from Pardisan Park, South-west of Tehran in April and in May 2002, respectively.

P-31

Essential oil composition from *Plagiochila retrorsa* Gottsche and *P. spinulosa* (Dicks) Dum. grown on Madeira

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The genus *Plagiochilla* comprises over 400 species, being one of the largest of the liverwort genera. *P. retrorsa* occurs in Central America and in the Southern Appalachian mountains of the eastern U.S.A. It is also known from the Azores and Madeira Archipelagos, in the Macaronesia.[1] In Madeira Island, *P. retrorsa* is a widespread species especially in the less humid parts of the native laurel forest where it can be found on rocks and slopes. *P. spinulosa* is quite common in the western Europe.[2] It is also frequent species in the Macaronesia, particularly on Madeira Island, where it grows on rocks and slopes covered with soil, along rivulets, tree trunks and branches. The essential oils of both species were isolated from deep-frozen plant material by distillation-extraction and analysed by GC and GC-MS.

The essential oil isolated from *P. retrorsa* was dominated by the monoterpene fraction (58%), β-phellandrene (46%) being the main component of the oil. Peculiaroxide (9%), bicyclogermacrene (6%), *allo*-ocimene (5%), *neo-allo*-ocimene (4%) and methyl everninate (4%) were the other main components (4%) of the oil. β-Phellandrene was also the dominant monoterpene identified by Rycroft *et al.*[1] on the solvent extracts of twelve collections of this species. Among the other main components these authors also detected peculiaroxide and bicyclogermacrene. According to Rycroft *et al.*,[1] *P. retrorsa* belongs to the 9,10-dihydrophenantrene chemotype due to the dominant components, 3,5-dimethoxy-9,10-dihydrophenanthren-2-ol and 4-hydroxy-4'-*O*-methyllunularate. However, these two compounds were not extracted on the essential oil from this species.

Methyl everninate (35%) and peculiaroxide (15%) were the dominant components of the essential oil isolated from *P. spinulosa*. β-Phellandrene (3%) and bicyclogermacrene (2%) were also present in this oil, but in a lower relative amount, than that found for *P. retrorsa*. *allo*-Ocimene and *neo-allo*-ocimene were not detected in this oil, but several other monoterpenes were present in relative amounts <0.1%. In common with Rycroft *et al.*[3] β-phellandrene was the main monoterpene from this population of *P. spinulosa*. Inoue and Asakawa[4] and Connolly *et al.*[5] reported the phytochemical analysis of the solvent extracts from this species collected in Belgium and Scotland, respectively. Inoue and Asakawa[4] identified α-pinene, bicyclogermacrene and spathulenol, and the remaining components were classified as sesqui- or diterpenes only. Connolly *et al.*[5] have studied the nonterpenoid constituents of *P. spinulosa*, 9,10-dihydro-3,4,7-trimethoxyphenanthren-2-ol methyl being the main component of the solvent extract. This compound was not extracted on the essential oil, but two other aromatic compounds were, 6-hydroxy-2methyl-3,4-methylenedioxybenzoate (3%) and methyl 6-methoxy-2methyl-3,4-methylenedioxybenzoate (0.3%).

Acknowledgements: This study was partially funded by the Fundação para a Ciência e Tecnologia (FCT) under research contract POCTI/AGR/42501/2001.

1. Rycroft D. S., J. Heinrichs, W. J. Cole, H. Anton (2001) *Journal of Briology*, 23: 23-34.
2. Paton, J. A. 1999. The liverwort flora of the British Isles. Harley Books. Colchester. 626p.

3. Rycroft D.S., W.J. Cole, J. Heinrichs, H. Groth, C. Renker, T. Pröschold (2002) *The Bryologist* 105: 363-372.
4. Inoue H, Y. Asakawa (1988) *Bull Nat. Sci. Mus., Tokyo*, Ser B, 14: 143-147.
5. Connolly J. D., D. S. Rycroft, D. L. Srivastava, W. J. Cole, P. Ifeadike, S. F. Kimbu, J. Singh, M. Hughes, C. Thom, U. Gerhard, A. J. Organ, R. J. Smith, L. J. Harrison (1999) *Phytochemistry* 50: 1159-1165.

P-32

Adrenergic Activity of the Essential oil of *Cymbopogon schoenathus ssp. proximus*

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Cymbopogon schoenanthus ssp. proximus Family Poaceae is known Sudan as Mahereb is a well-known aromatic and medicinal plant (Broun and Massi, 1929). In Sudan the aerial parts are used as antispasmodic and for treatment of stomach and kidney pain. The present work aimed to verify or refute the claimed activity. The hydrodistilled oil was emulsified using Ethylene Glycol as emulsifying agent. The emulsion was studied in Rabbit jejunum isolated tissue. The results showed a significant dose dependant inhibition, which was not observed when using the Polyethylene Glycol alone.
The relaxant activity of the oil was completely blocked by prior administration of the non-selective ß-antagonist "Propanalol".
This result indicates the adrengenic selective ß-agonist effects of the oil and suggests further investigation to specify the ß-adrenoreceptor subtypes the oil activates.

Reference

Broun, A. F. and Massey, R. E. (1929) Flora of Sudan, Thomas Murby and Col. Fleet Lane E.C.4. 1929.

P-33

Essential oil composition from the leaves of *Meum athamanticum* Jacq. from Spain

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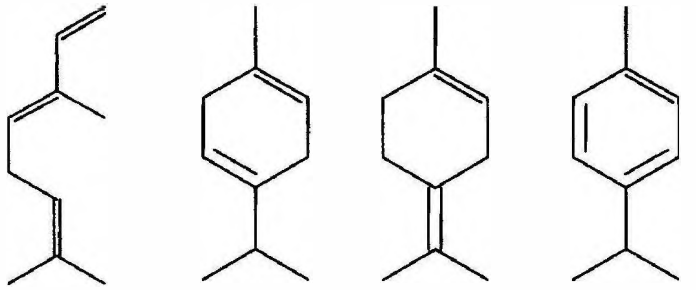
The genus *Meum* Miller belongs to the Umbelliferae family, one of the most widely distributed around the world. *Meum athamanticum* Jacq. is the only species belonging to this genus growing in Spain (1).

The essential oil of the leaves from *M. athamanticum* has been extracted by steam distillation and analysed by Gas Chromatography (GC) and Gas Chromatography coupled to Mass Spectrometry (GC-MS). Although we have found previous reports about this species (2-4) we have found a different chemical composition from the Spanish species analysed. The monoterpenoid fraction was predominant while the sesquitepenoid one was practically absent. The principal constituents have been identified as (*E*)-*Z*-ocimene (29.6%), γ-terpinene (17.9%), terpinolene (17.0%) and *p*-cymene (9.7%).

Main constituents



(*E*)-β-ocimene γ-terpinene terpinolene p-cymene

1. Flora Europaea, Vol. 2. 1968. Edited by T.G. Tutin, V.H. Heywood, N.A. Burges, D.H. Valentine, S. M. Walters and D.A. Webb. Cambridge at the University Press.
2. B. Tirillini, R. Pellegrino, A. Menghini and B. Tomaselli. 1999. Essential oil components in the epigeous and hypogeous parts of *Meum athamanticum* Jacq. Journal of Essential Oil Research. **11**, 251-252
3. K.H. Kubeczka, V. Formacek and M Grünsfelder. 1980. The essential root oil from Meum athamanticum. Planta Medica. **39**, 271.
4. K.H. Kubeczka, A. Bartsch and I. Ullmann. 1982. Recent investigation of essential oils of Apiaceae. In: Essential Oils, Analysis, Physiology, Composition. Edit., K.H. Kubeczka 158-187. Georg Thieme Verlag Stuttgart. New York.

P-34

Constituents of the bark essential oil of *Cedrelopsis grevei* Baill, an aromatic and medicinal plant from Madagascar

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Among the eight species of the genus *Cedrelopsis* (Ptaeroxylaceae), all native to Madagascar, *Cedrelopsis grevei*, is the most exploited on the island not only for its wood but for its medicinal properties as well. The whole plant (leaves, stems, bark, seeds) is indeed widely used in folk medicine in various ways : decoction, infusion, powder mixed with lard or essential oil. The bark essential oil in particular is used as fortifying, tonic, postnatal medications and to relieve rheumatism and muscular pains. It is also reported to exert antifungal and antibiotic activities. Because of these various medicinal properties, we decided to analyse the volatile constituents of the bark essential oil commercially available not only in Madagascar but in France and South Africa as well.

The gas chromatography - mass spectrometry analysis resulted in the identification of fifty-seven components representing 84.7% of the oil. Sesquiterpene hydrocarbons were the principal constituents (57.2%) including 10.6% of β-caryophyllene, 10.2% of α-copaene, 9.2% of β-bisabolene and 8.7% of ar-curcumen. The monoterpene hydrocarbons (17.1%) and the oxygenated containing sesquiterpenes (7.7%) were the two other main fractions of the oil. At last, oxygenated monoterpene derivatives were found in very small amount (1.8%).

P-35

Sesquiterpenes and other constituents of the liverwort *Plagiochila killarniensis*

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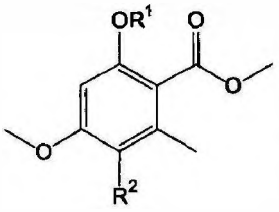
The essential oil of the liverwort *Plagiochila killarniensis* from Madeira has been investigated by GC and GC/MS, leading to the identification of 38 known compounds. These include some aromatic compounds, methyl everninate (**1**) as the major component and four minor methyl orsellinate derivates (**2** – **5**), which were previously identified in *P. killarniensis* from Scotland and the Azores by Rycroft *et al.* [1] Chemical similarity is also shown by the presence of formerly detected terpenes, β-phellandrene, germacrene D, bicyclogermacrene and fusicoccadiene and some other constituents which were presented by their mass spectral data but remained unidentified.

Three of these formerly unidentified compounds could be isolated in this work along with another minor component and were identified as peculiaroxide (**6**) [2], *ent*-eudesm-4-en-6-one (**7**), *ent*-eudesm-4(15)-en-6-one (**8**) and *ent*-7-hydroxyeudesm-4-en-6-one (**9**). Compounds **7** - **9** are described for the first time as constituents of liverworts, although they were previously isolated from a higher plant in their enantiomeric form [3]. The structure of these sesquiterpenes has been determined using standard NMR experiments. Their absolute configuration was assigned by chemical correlation and enantioselective gas chromatography.



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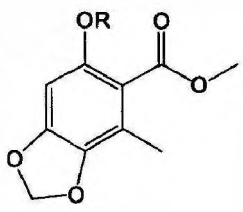
3: R^1 = Me, R^2 = OMe



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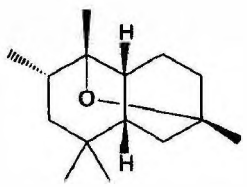
5: R = Me



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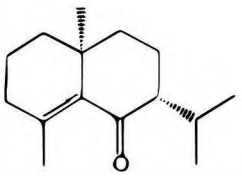

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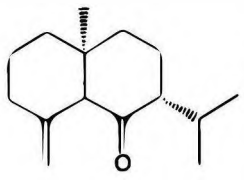

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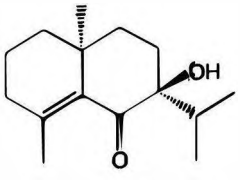

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[1] D.S. Rycroft, W.J. Cole, N. Aslam, Y.M. Lamont, R. Gabriel, (1999) *Phytochemistry*, **50**, 1167-1173.
[2] C.-L. Wu, C.-D. Huang, T.-L. Shih, (1993) *Tetrah. Letters*, **34**, 4855-4856
[3] J. Kawabata, Y. Fukushi, S. Tahara, J. Mizutani, (1985) *Agric. Biol. Chem.*, **49**, 1479-1485.

P-36

Study of essential oils composition from *Origanum dictamus* at different storage conditions

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Essential oil from fresh and dried O*riganum dictamus* were obtained. Samples from the same area and different harvesting time were treated by steam distillation. Gas Chromatography (GC) and Gas Chromatography–Mass Spectrometry (GC-MS) were used to determine the different compounds in the essential oils. However, yield was also determined and used as the first aproch in this document.

Results show that the chemical composition of essential oils depends on different parameters, such as the enviromental conditions, the harvesting time, the stortage conditions under which the collected plants were kept until the time of extraction. Relative high yield ratio were observed among the different seasons, moreover the lowest value was observed in winter and the highest one in summer. *Carvacrol* showed to be the main compound found in all the samples studied.

P-37

The essential oil composition of linaloe oil (*Bursera delpechiana*)

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Linaloe oil is produced mainly in Mexico from the wood and, to a small extent, from the fruit, of the linaloe tree (*Bursera delpechiana* Poisson) (1). Linaloe oil may be used in the same ways as rose wood and ho leaf oil and has in recent years been replaced by those oils. A sample of linaloe oil was obtained from Aromatica (Turku, Finland), a small company specialised in aromatherapy oils, and studied by GC-MS. 22 components accounting for 97.2% of the oil were identified. The main component was linalool (81%). Also linalool oxides, citronellol, nerol, geraniol and geranyl acetate were detected.

1. Guenther, E, The Essential Oils, D. van Nostrand Company Inc., New York 1950, pp. 331-344.

P-38

Chemical Composition of the Essential Oils of *Citrus hystrix* (Rutaceae) Leaves, Fruits and Peels of Thailand

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Kaffir lime (*Citrus hystrix,* Rutaceae) is a native plant in Asia. Especially in Thailand, kaffir lime is utilized for various medical and culinary uses. The essential oils from *Citrus hystrix* leaves, fruits and peels were investigated in this study. The essential oils were extracted by hydrodistillation in a Clevenger apparatus. The distillation time was 3 hours. The means of obtained oils were 0.51 % for fruits, 1.50 % for peels and 0.83 % for fresh leaves. Three drying treatments with leaves were employed: air-drying at 25°C for 10 days, oven-drying at 40°C for 6 hours and freezing at -20°C for 24 hours. The essential oils were analyzed by Gas Chromatography (GC) and Co-chromatography. The main volatile components were different in various parts of the *Citrus hystrix.* Four main components, i.e. beta-pinene, limonene, citral and terpinene-4-ol, were prominent in the essential oil of kaffir lime fruits. As main constituents of kaffir lime peels also beta-pinene, limonene and citronellal were found. The most abundant component of kaffir lime leaves was only citronellal.

P-39

Chemical constituents of the volatile fractions from leaves and flowers of *Ocimum urticifolium* Roth

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Volatile fractions from leaves and flowers of the native African plant *Ocimum urticifolium* Roth (1-4) were obtained by steam distillation and analyzed by gas chromatography (GC) and gas chromatography–mass spectrometry (GC–MS). Twenty-seven compounds, representing 89.0 % of the volatile fraction from the leaves were identified, while fifty-five compounds, representing 63.9 % of the volatile fraction were identified in the flower essential oil. The main sesquiterpene constituent found in the leaves was δ-cadinene (17.2 %) together with β-caryophyllene (14.5 %) and γ-muurolene (10.5 %). The dominant monoterpene compound of the leaves was (*Z*)-β-ocimene (22.7 %), while the biologically active phenylpropanoid elemicine was detected by 8.8 %. The main sesquiterpene compound detected in the flowers was β-bisabolene (19.2 %) followed by β-caryophyllene (10.5 %). The major monoterpene in the flowers was linalool (2.3 %) which was found to be present together with (*Z*)-β-ocimene (2.4 %) and camphor (1.5 %). High amounts of elemicine (6.4 %) could also be detected in the flower essential oil. A higher number of monoterpene and sesquiterpene constituents were detected in the flowers compared to the leaves. The yield of the essential oil was 0.48 % and 0.21 % (v/w) for flowers and leaves, respectively.

References

(1) Ayobangira FX, Ntezurubanza L. 1987. Morphological and chemical variations in *Ocimum urticifolium* Roth equals *Ocimum suave* Willd. in Rwanda. Taxonomic significance of these observations. *Plantes Medicinales et Phytotherapie* **21**:236-241.

(2) Chagonda LS, Makanda CD, Chalchat JC. 2000. The essential oils of *Ocimum canum* Sims (basilic camphor) and *Ocimum urticifolia* Roth from Zimbabwe. *Flavour Frag J* **15**:23-26.

(3) Ntezurubanza L, Scheffer JJC, Svendsen AB. 1988. Composition of the essential oils of *Ocimum urticifolium* (Lamiaceae) chemotypes grown in Rwanda. *Bot J Linn Soc* **96**:97-104.

(4) Yirdaw, E. 2002. Restoration of the native woody-species diversity, using plantation species as foster trees, in the degraded highlands of Ethiopia. PhD Thesis, University of Helsinki, Finland, 61p.

P-40

Study and comparison of the essential oils of three *Stachys species* grown in Iran

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Stachys is one of the important genus in Lamiaceae family. It is represented by thirty-one species in the flora of Iran which eighteen of them are endemic species. Plants of this genus have been reported to be used to treat genital tumors, inflammatory tumors and cancerous ulcers in folk medicine. Methanolic extract of tuber of *S. sieboldii* presented anti-anoxia action in mice and hydroalcoholic extract of aerial parts of *S. inflata* showed potent anti-inflammatory activity in rats.

Water distilled essential oils from aerial parts of *S. obtusicrena, S. pilifera* and S. *lavandulifolia* were analyzed by GC and GC-MS. The compounds were identified by comparison of retention indices with those reported in the literature and by comparison of their mass spectra with the Wiley library or with the published mass spectra. Eighty-three compounds were identified representing 85.9% of the essential oil of *S. obtusicrena*. The main components were spathulenol (11.5%) and 10-epi-γ-eudesmol (6.8%). In *S. pilifera*. the main components of the oil were spathulenol (15.8%), cis-chrysanthenol (15.3%), E-caryophyllene (8.4%) and cis-chrysanthenyl acetate (6.9%). In S. *lavandulifolia* oil seventy-three compounds were identified representing 96.7% in the essential oil in which the major components were pulegone (26.5%), piperitenone oxide (17.4%) and α-terpinyl acetate (11.2%). As can be seen in the above information, the oil of *S. obtusicrena* was rich in sesquiterpenes, while S. *lavandulifolia* oil was mainly consisted of oxygenated monoterpenes and *S. pilifera* was rich in both of them (sesquiterpenes and oxygenated monoterpenes).

P-41

Volatile constituents from *Siraitia grosvenorii* dried fruit

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The dried fruits of *Siraitia grosvenorii* (Swingle) C. Jeffrey, have been known since ancient times in China for their intense sweetening effect. In addition to this property, which finds applications in low-calorie foods, other features such as antiradical activity makes extracts of this fruit attractive as *nutraceutical* and *cosmeceutical* ingredients. However, the characteristic flavor of the dried fruit, which is reminiscent of licorice, has not been studied so far. We report herein the composition of the volatile fraction, which was analyzed on a single fruit by SPME-GC-MS, and SPME-PFPD-GC, using different adsorbing fibers and GC stationary phases. The main flavor-donating elements have been found to be 2-acetylpyrrole and a number of 2-methylalkylcarbinols, and esters including unusual crotonates.

P-42

Combinatorial QSAR for Ambergris Fragrance Compounds

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QSPR models are typically generated with a single modeling technique. We have developed a combinatorial QSAR approach which explores all possible combinations of various descriptor sets and optimizations methods coupled with external model validation. This approach was explored using a set of 98 ambergris fragrance compounds. Descriptor sets included Topological Indices (TI), MOE, CoMFA, CoMMA, Dragon, Volsurf and 2D-chirality descriptors recently developed in our laboratory. Optimization methods included kNN-classification, Support Vector Machines (SVM), decision tree and binary classification.
The models were considered to be acceptable if they had both high internal accuracy for the training set and external prediction power for the test set. The best model had internal and external accuracy of 74% and 85%, respectively.
The combinatorial QSAR approach is automated, efficient, and affords selection of robust models with validated prediction power.

P-43

Volatile Compounds in Roasted Italian Chestnuts (*Castanea sativa*)

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Unlike most other tree nuts, chestnuts (*Castanea*) are low in fat content but high in carbohydrate (1-5). Nevertheless, it seems that this fruit is an interesting source of essential fatty acids (mainly linoleic), which play, an important role in preventing cardiovascular diseases and in promoting the development of the brain and retina of infants. From a nutritional point of view, chestnuts used to be a stable food in the southern valleys of the Swiss, Italian and French Alps (5).
Historically, the chestnut tree had a deep influence on the human progress and on the formation and growth of the agricultural landscape (6). The first cultivar breeds grew up in Minor Asia and spread out over the Hellenic peninsula from which, at the Magna Greec Time, they reached Italy (7). In Europe the chestnut spread from South to North, from Mediterranean to Sweden, thanks to farmer's intervention. In particular, the mountain man always lived in symbiosis with the chestnut. He set up a new village only where the chestnut could grow and give fruits (6).
Today beyond the classical transformations of chestnuts (roasted or candied chestnuts, chestnut puree or creams), new commercial products have been launched on the market (liqueur, aperitif, beer, pasta, dairy products) and it is now even easy to find vacuum-packed or frozen chestnuts (8).
Although numerous investigations have been carried out with respect to the constituents of chestnuts, very little was known yet about the volatile components of roasted chestnuts (*Castanea sativa,* Mill) and thus on the unique and very appreciable flavour.
In this work Solid Phase Micro Extraction (SPME) with DVB-Carboxen-PDMS fiber and GC-MS were used to obtain the chromatographic profile of chestnut volatiles.
3-Penten-2-one, hexanal, 2-furan-carboxaldehyde, hexanol, 2-heptanone, 3-hepten-2-one, benzaldehyde, 2-pentylfurane, octanal, acetic acid-hexylester, alpha-terpinene, p-cymol, limonene, gamma-terpinene, alpha-terpinolene, terpinen-4-ol and carvon have been identified as main volatile compounds of roasted Italian chestnuts.

1 McCarthy M.A. and Meredith F.I., Nutrient data on chestnuts consumed in the United States. *Econ. Bot.* **42**: 29-36 (1988)
2 Senter S.D., Payne J.A., Miller G. and anagnostakis S.L., Comparison of total lipids, fatty acids, sugars and nonvolatile organic acids in nuts from *Castanea* species. *J. Sci. Food Agric.* **65**: 223-227 (1994)
3 Morini G. and Maga J.A., Changes in the fatty acid composition of roasted and boiled Chinese (*Castanea molissima*) and Italian (*C. sativa*) chestnuts grown in the same location, in *Food Flavors: Generation, Analysis and Process influence.* Ed by Charalambous G., Elsevier science, Amsterdam, pp 563-568 (1995)
4 Künsch U., Schärer H., Patrian B., Hurter J., Conedera M., Sassella A., Jerimini M. and Jerimini G., Quality assessment of chestnut fruits. *Acta Hort* **494:** 119-127 (1999)
5 Künsch U., Schärer H., Patrian B., Höhn E., Condera M., Sassella A., Jermini m. and Jelmini G., Effects of roasting on chemical composition and quality of different chestnut (*Castanea sativa* mill) varieties. *Journal of the Science of Food and agriculture* **81**: 1106-1112 (2001)

6 Adua M., The sweet chestnut throughout history from the miocene to the third millennium. *Second International Symposion on Chestnut*, Bordeaux, 19-23 October 1998. 29-36 (1998)
7 Adua M. Sweet chestnutproduction and marketing in Italy. *Second International Symposion on Chestnut*, Bordeaux, 19-23 October 1998. 49-54 (1998)
8 Gloaguen V., Nourani D., Morvan H., Chestnut envelopes contain Xylan- and Polygalacturonicacid-rich Polysaccharides, *Second International Symposion on Chestnut*, Bordeaux, 19-23 October 1998. 139-142 (1998)

P-44

Separation of water soluble essential oil components by SPE

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For the evaluation of the physiological effects of terpenes but also for controlling the correctness of the essential oil analyses, the knowledge of the water solubility of essential oil components is of special importance. With classical solvent extraction or with SPME usually only small water samples can be examined. With the help of the equipment in fig.1 it is possible to extract the entire distilled water of an analytic hydrodistillation. The distilled water with the solved oil components is pumped off by a flow inducer at the refill fitting of the distillation apparatus. Water and solved components are led over a RP18-SPE-cartridge. The solid phase retains the oil components, the water flows back into the flask.

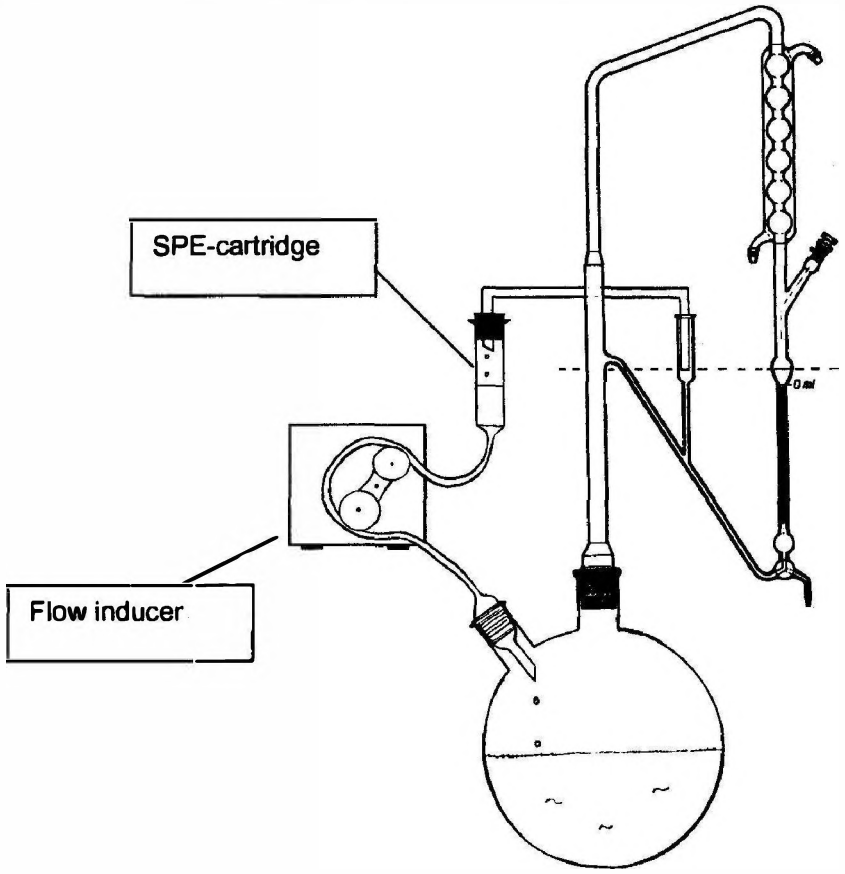

Fig. 1: Equipment for the separation of water-soluble essential oil components

After elution (n-hexane/acetone: 90/10) the components solved in water can be investigated by GC. Particularly polar substances such as phenols from *Thymus, Origanum* or *Satureja* or alcohols from *Ocimum* or majoram were isolated and determined quantitatively.

P-45

Composition of the Essential Oil from *Laserpitium gallicum* L. Fruits

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Laserpitium gallicum L. belonging to the Apiaceae (Umbelliferae), subfamily Laserpitieae is a up to 120 cm calcicolous shrub, growing in the mountains of South Europe from Spain to Italy.

Phytochemical studies performed on the leaves and the roots led to the identification of sesquiterpene lactones (1,2), and flavonoids (3). Only one previous report concerning the chemical composition of the volatile constituents of *Laserpitium gallicum* fruits was found, which solely described the presence of α- and ß-pinene (60-64% and 26-38%, respectively) and small amounts of limonene and p-cymene (4).

We have therefore investigated the essential oil from the fruits, obtained by hydrodistillation in more detail by means of GC and GC-MS. In this oil 63 constituents mainly belonging to monoterpene hydrocarbons (78,4 %) and oxygenated monoterpenoids (13,4 %) were identified. Main constituents were as previously found α- and ß-pinene (32.6 and 33.5%), besides lower concentrations of limonene and sabinene (both 4.5 %). Only small amounts of sesquiterepene hydrocarbons (1,65 %) and oxygenated sesquiterpenes (1,34 %), and in addition some fatty acids (1.53 %) could be detected.

1. Holub, M. and Budešinský, M. (1986) *Phytochemistry* **25**, 2015
2. Appendino, G., Cravotto G. and Nano, G.M. (1993) *Phytochemistry* **33**, 883-886.
3. Crowden, R.K., Harborne, J.B. and Heywood, V.H. (1969) *Phytochemistry* **8**, 1963-1984.
4. Adcock, J.W. and Betts, T.J. (1974) *Planta Medica* **26**, 52-64.

P-46

Composition of the Essential oils of *Thymus caucasicus* Willd. ex Ronniger subsp. Grossheimii (Ronniger) Jalas and *Thymus nummularius* M.B. from Iran

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The genus Thymus include, 300-400 species and some species are used in folk medicine .The main medicinal Thymus are T. *vulgaris* (common thyme) and *T. serpyllum* (wild Thyme) that are used internally for dry coughs, bronchitis, laryngitis, indigestion and gastritis and externally for rheumatism, arthritis, sciatica and mastitis.
The oils obtained by hydrodistillation of the aerial parts of *Thymus caucasicus* and *Thymus nummularius*, which are endemic to Iran, were analyzed by GC and GC/MS.
Carvacrol (57.0%) and thymol (18.9%) were the main components among the twenty-eight constituents characterized in the oil of *T. caucasicus* representing 99% of the total components detected.
Twenty-seven components were identified in the oil of *T. nummularius* representing 97% of the total oil with dihydrocarveol acetate (54.8%) and carvacrol (10.6%) as major constituents. Both oils were rich in oxygenated monoterpenes.

P-47

Essential Oils from Western Canada

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Alberta's native plants produce a wide variety of essential oils, some of which may have considerable economic value. Essential oil production in Alberta is relatively small, however there is growing interest in cultivation of mint, dill and monarda. A data bank containing the chemical composition of essential oils from native and cultivated aromatic plants produced in Western Canada is being established. This database will help to establish quality control standards for Alberta's essential oils. For quality control purposes, the oils are obtained in a laboratory Clevenger-type distillation unit and a semi-commercial portable unit. Over 163 oils have been analyzed by gas chromatography- mass spectrometry using two different capillary columns (HP-5 and DB-Wax). The identification of single aroma components is being performed by comparison of retention indices, mass spectra and co-injection of authentic standards.

The other part of the project is the analysis of essential oils produced from Canadian coniferous trees. The yield and chemical composition of oils obtained from needles of Canadian conifer species (incense cedar, white spruce, Colorado spruce, giant sequoia, coast redwood, western red cedar, mountain hemlock, ponderosa pine, Douglas fir and Nootka cypress) will be described.

P-48

Solvent-Free Microwave Extraction: a Prospective Tool for Rapid Extraction of Essential Oils

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A new alternative for extracting natural products by using microwave energy has been developed and patented. Based on a relatively simple principle, this method involves placing plant material in a microwave reactor, in the absence of any solvent or water. The internal heating of water within the plant material distends it and makes the glands and oleiferous receptacles burst. This process thus frees essential oil which is evaporated by the ***in situ*** water of the plant material. The SFME extractions have been performed in a Milestone ETHOS 1600. During experiments, time, temperature, pressure, and power were monitored/controlled with the "easy-WAVE" software package. Microwave power applied to the sample is controlled by a non-contact infrared sensor and/or a shielded thermocouple inserted directly into the container.

The solvent free microwave extraction (SFME) is a new extraction system consisting on an atmospheric pressure microwave assisted dry distillation for essential oil extraction from aromatic plant materials or dry seeds. SFME is not a modified microwave assisted extraction (MAE) which use polar or non polar solvents. It is neither a modified hydro-distillation which use not only large quantity of water, but it is also known to be time and energy consuming.

The essential oils from aromatic herbs (basil, crispate mint, thyme) and spices (ajowan, cardamom, cumin, star anis) extracted by SFME for respectively 30 minutes and 1 hour, was quantitatively and qualitatively identical with that obtained by conventional hydro-distillation for respectively 3 and 6 hours. The SFME is clearly advantageous in terms of rapidity, efficiency, cleanliness, substantial saving of energy, and is environmentally friendly. This green technology appears as a good alternative for the extraction of essential oils from aromatic plants or spices.

P-49

Volatile Constituents of *Ferulago phialocarpa* Rech.f.& H . Riedl . and *Leutea elbursensis* Mozaffarian. Two Umbelliferae Herbs Growing Wild in Iran

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The water distilled volatile oils from aerial parts of *Ferulago phialocarpa* Rech. f. & H. Riedl. and aerial parts of *Leutea elbursensis* Mozaffarian, two Umbelliferae species, which are endemic to Iran, were analyzed by GC and GC/MS.

α-Pinene (40.9%), α-phellandrene(14.2%) and β-phellandrene (9.6%) were the main components among the 26 constituents characterized in the oil of *Ferulago phialocarpa*, represented 93.8% of the total components detected.

The oil of *F. phialocarpa* was characterized by large amounts of monoterpene hydrocarbons (88.8%), lesser amount of oxygenated monoterpenes and sesquiterpenes (1.3% and 3.7% respectively).

Thirty-three compounds were identified in the oil of *Leutea elbursensis* representing 98.0% of the total oil with α-pinene (37.3%) and β-pinene (36.1%) as main constituents.

The oil of *L. elbursensis* was characterized also by high amounts of monoterpene hydrocarbons (85.9%). The sesquiterpene fraction was relatively small, representing only 0.2% of the total oil.

The aerial parts of *F. phialocarpa* were collected during the flowering period from Divandareh to Saghez , Province of Western Azarbaijan, Iran, in July 2000, and the aerial parts of *L. elbursensis*, a newly discovered wild *Leutea* in Iran, were collected in Karaj area, 35 Km. North of Tehran, in June 2000, during the flowering stage.

P-50

Chemical and Microbiological Investigations of Thyme Oil Cultivated in Iran and Its Application in Toothpaste and Shampoo

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Thyme is one of the most important plants that is used widely in pharmaceuticals and cosmetics, in Iran it is called Awishan. The dried leaves and flowering tops of plant contain 0.8-2.6 % essential oil and the main components of the oil are thymol and cacvacrol.
This research was performed to investigate the quality and quantity of the essential oil of the *Thymus vulgaris* L. cultivated in Iran and Iranian Thyme *Zataria multiflora* Boiss. The essential oils of the plants were obtained with hydrodisstilation method by a cleavenger apparatus for 4 hours and the components of the essential oils were determined by GC. We studied the antibacterial effects of the essential oils, thymol, hydroglycolic extract and infusion against some of Gram positive and negative bacteria. The minimal inhibatory concentration determined according to the UCCSL Protocol.
Finally several toothpastes and shampoos containing essential oils, thymol, hydroglycolic extract and infusion were formulated, without preservative, to study inhibatory effects of them.
Our experiments showed that all of toothpastes and some of shampoos had positive effects.

P-50a

Structural requirements of olfactory receptors for the specific recognition of odours

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The olfactory system can recognize and discriminate numerous structurally diverse odour molecules through binding of these fragrances to G- protein-coupled olfactory receptors (ORs). The mouse olfactory receptor repertoire comprises 930 functional ORs, whereas humans possess only 300 functional ORs, the remaining 700 receptors being pseudogenes.

There is very limited information on molecular level about the binding mechanism of odorants to ORs, particularly how this leads to activation or inhibition of the corresponding receptor. One of the major problems is that despite of years of intense effort no crystal structure information of any olfactory receptor exists. Therefore, structural information of ORs can only be acquired by computational modelling techniques.

Another outstanding problem is the assignment of the large repertoire of volatile chemicals to the receptor repertoire. Up to now, less than 1% of OR – ligand couples from different species have been identified, leaving the vast majority of olfactory receptors semi-orphan, since their specificity is unknown.

Since knowledge of the three-dimensional structure of ORs is crucial for the interpretation of functional data, we concentrated on developing computational techniques suitable for predicting the structure of olfactory receptors, simulating the ligand receptor interaction and the activation mechanisms of ORs in general. The study focuses on the olfactory receptors OR1D2, OLFR43, OLFR16 and OR3A1, which recognize some identical fragrance molecules with distinct affinities. Starting from multiple sequence alignments consensus sequences were calculated, providing a general idea of specific key amino acids, necessary to receive the odour impression elicited by the floral fragrances Helional® and Lilial®. Three dimensional structure models were built using bovine rhodopsin as template. Molecular dynamics simulations of the models embedded in a lipid bilayer surrounded by a water box were performed to check the stability of the receptors, followed by molecular docking simulations. These studies shed some light on the receptor – ligand interactions. Our studies prove the existence of conserved structural binding site features even between distant related olfactory receptors. In the case of Helional® D183, Y262 and T282 were identified as key residues, necessary for specific recognition. However, there most likely exist additional important amino acids, which can be found comparing larger data sets of olfactory receptors, recognizing this fragrance molecule. Generally knowledge of larger numbers of receptor – ligand pairs will shed light on how the olfactory receptor family has evolved the ability to recognize such a variety of distinct chemical structures.

P-51

Evaluation of the antioxidant activity of the essential oils of *Origanum vulgare* and *Thymbra capitata* by different methodologies

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The use of natural antioxidants for improving the antioxidant stability of food lipids has received more and more attention in order to replace the synthetic antioxidants believed to possess carcinogenic activities. Aromatic plants and their essential oils have been target of some antioxidant activity studies. Several analytical methods can be used for determining the extent of oxidation of a food lipid, rendering many times difficult to compare and to interpret the effectiveness of the antioxidant used. The lipid oxidation is a multiple step therefore it is important to analyze the action of a potential antioxidant on the different steps of the oxidation process.

In the present work the composition and the antioxidant capacity of the essential oils of *Origanum vulgare* and *Thymbra capitata*, collected during the flowering phase, from plants grown on Algarve was evaluated. The antioxidant capacity was assayed using two methods for the primary oxidation products determination (peroxide value conjugated diene hydroperoxides) and two methods for the secondary oxidation products determination (malonaldehyde and anisidine).

The highest antioxidant values, for both *O. vulgare* and *T. capitata* oils, were obtained when the antioxidant capacity was measured by the malonaldehyde and conjugated diene hydroperoxides detection methodologies. With malonaldehyde detection methodology the antioxidant effectiveness of the essential oil of *T. capitata* ranged from 68%, at 160ppm, to 86%, at 800ppm. Similar results were obtained with the essential oils of *O. vulgare* (79% to 87% at 160ppm and 800ppm, respectively). The determination of the rate of conjugated diene hydroperoxides formation also proved the protective capacity of those essential oils as inhibiting the peroxidation of linoleic acid.

Although the antioxidant capacity of an oil can not be exclusively attributed to its main component, the high amount of the phenolic compounds carvacrol (76%) for the oil of *T. capitata* and thymol (33%) for the oil of *O. vulgare*, can partly be responsible for their activities.

P-52

Antioxidant activity of essential oils isolated from some Portuguese native *Thymus* plants

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Several reports have demonstrated the chemical composition and variability of the essential oils isolated from *Thymus* species collected in Portugal (1). Nevertheless, their antioxidant properties only very recently have been described (2). In the present work the antioxidant activity of *Thymus mastichina*, *T. albicans*, *T. camphoratus* and *T. carnosus* essential oils, at different concentrations, were evaluated and compared to those generally used in Food Industry (BHT, BHA and tocopherol). Antioxidant activity was measured through the modified thiobarbituric acid reactive species (TBARS) assay, using egg yolk as lipid-rich media. The chemical composition of the essential oils, isolated by hydrodistillation, was studied by GC and GC-MS.

T. mastichina essential oil was dominated by 1,8-cineole (60 %) while that of *T. albicans* had also high percentages of 1,8-cineole (44 %) along with linalool (15 %). *trans*-Sabinene hydrate (23 %), terpinen-4-ol (9 %) and sabinene (7 %) were the major components of the oils isolated from *T. camphoratus*. The essential oil of *T. carnosus* was mainly composed by borneol (23 %), *cis*-sabinene hydrate (16 %) and camphene (12 %).

In the absence of the radical inducer ABAP, *T. camphoratus* and *T. carnosus* oils showed the highest antioxidant activity (49 % to 78 %), regardless the concentrations tested. This activity was always lower than that found for BHA (60-80 %) and BHT (81-84 %). In the presence of ABAP, the antioxidant ability of the *T. carnosus* oil was significantly higher (39-74 %) than the remaining oil samples, but still lower than α-tocopherol (93-97 %), BHT (82-90 %) and BHA (90-97 %).

1. Salgueiro, L. R. (1994) Doctoral Thesis, Vol. 1. Faculty of Pharmacy, University of Coimbra, Portugal.
2. Miguel, M. G.; Figueiredo, A. C.; Costa, M. M.; Martins, D.; Duarte, J.; Barroso, J. G.; Pedro, L. (2003) Nahrung/Food (accepted).

P-53

Analysis of the volatile constituents of *Nepeta macrosiphon* Boiss. and *Nepeta ucrainica* L. ssp. *kopetdaghensis* from Iran

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The genus *Nepeta* (Lamiaceae) comprises about 280 species in the world and forty-two species endemic in Iran. *Nepeta cataria* (catnip) has been used as a calmative and sleep aid. The essential oil components of catnip, nepetalactone has sedative effects which makes it useful migraine headaches, nervous disorders and digestive complaints. Two essential oils of *N. camphorata* and *N. argolica* ssp. *dirphya* showed some activity against *Helicobacter pylori*.

Composition of the volatile oil of *N. macrosiphon* and *N. ucrainica* was investigated by GLC and GC-MS The compounds were identified by comparison of retention indices with those reported in the literature and by comparison of their mass spectra with the Wiley library or with the published mass spectra. Seventy-three components representing 96.9% of the total oil were characterized in the oil of *N. macrosiphon*. The main components of the oil were spathulenol (28.8%), α-cadinol (13.6%), bicyclogermacrene (10.1%), β-caryophyllene (9.6%) and linalool (5.6%). . Forty-one compounds represent 89.5% of the oil of *N. ucrainica* were identified. The main components of the oil were germacrene-D (39.7%), palmitic acid (10.8%), β-bourbonene (5.8%), and spathulenol (5.6%). The oils were rich in sesquiterpenes and Nepetalactone isomers were not present in these two essential oils.

P-54

Identification of the Essential Oil of *Salvia sharifii* Rech. f. & Esfand from Iran

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The essential oil isolated by steam distillation from aerial parts of *Salvia sharifii* Rech. f. & Esfand growing wild in Iran was analyzed by GC and GC/MS.
Its mean oil content was 0.1% (w/w). Twenty-five components were identified in the oil, representing approximately 99% of the oil. The oil of *Salvia sharifii* is dominated 92 % by sesquiterpenes. In particular, the oil of this species is characterized by a high content of â-caryophyllene (36.9%), germacrene-D (26.7%), and bicyclogermacrene (11.6%).
Ten monoterpenes were identified which their contents ranging from 0.1 to 3.5% in the oil analyzed. Other compounds present in apreciable amounts are spathulenol (5.0%), caryophyllene oxide (3.4%), α-humulene (1.9%), ß-eudesmol (1.6%), ß-elemene (1.3%), limonene (1.2%), and α-copaene (1.0%).

References

1. Mozaffarian V. *A Dictionary of Iranian Plant names*, Farhang Moaser, Tehran, 1996, p 407.
2. Hooker J D and Jackson B D. *Index Kewensis*, Oxford at the Clarendon Press, 1960, vol **2.**
3. Zargari A. *Medicinal plants*, Tehran University publisher, 1990, *, p 150
4. Sandra Pand, Bicchi C. *Capilary Gas Chromatography in Essential Oil Analysis,* Alford Huethig Verlag: New York, 1987.

P-55

Volatile constituents of *Bothriochloa ischaemum* (L.) keng from Iran

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The oil obtained by steam distillation of the aerial parts of *Bothriochloa ischaemum* (L.) keng (Gramineae) growing wild in Iran, were investigated by a combination of GC and GC/MS. 13 compounds in the oil have been identified representing 92 % of the oil. The main constituents were, viridiflorol (73%), valencene (3.5%) and ß-selinene (3.1%). The yellow essential oil of *B. ischaemum* was obtained in a yield of 0.08 % (w/w), based on the dry weigh of the sample.

References

1. Sandra P, Bicchi C. *Capillary Gas Chromatography in Essential Oil Analysis,* Alford Huethig Verlag: New York, 1987
2. Adams, RP. *Identification of Essential Oils by Ion Trap Mass Spectroscopy.* Academic Press: San Diego, CA, 1989.
3. Mozaffarian V. *A Dictionary of Iranian Plant names*,Farhang Moaser, Tehran, p 407 , 1996.
4. Hooker J D and Jackson B D. *Index Kewensis,* Oxford at the clarendon press, 1960 vol 1.

P-56

High performance liquid chromatographic method for the determination of (–)-verbenone 10-hydroxylation catalyzed by rat liver microsomes

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A sensitive assay for the determination of (–)-verbenone 10-hydroxylation catalyzed by rat liver microsomes was developed using high-performance liquid chromatography. Verbenone was incubated *in vitro* with liver microsomes of untreated rats and rats treated with phenobarbital and the products thus formed were extracted with CH_2Cl_2 and the extracts were separated by HPLC with a C_{18} 5-μm analytical column. Elution was conducted with 40% methanol containing 20 mM $NaClO_4$ and the detection of UV absorbance was done at 251 nm. Product formation was dependent on the incubation time at least up to 30 min and the microsomal protein concentration between 0.01 and 0.1 mg protein/ml. The limit of detection of (–)-10-hydroxyverbenone with the HPLC was found to be about 40 pg, indicating that this method is about 100-fold sensitive than the GC-MS method. Optimized pH for the reaction was at 7.4 when examined with 100 mM potassium phosphate buffer in different pHs. Kinetic analysis showed that K_m values for liver microsomes of untreated and phenobarbital-treated rats were 206 and 41 μM and V_{max} values were 5.8 and 44 nmol/min/mg protein, respectively. Thus the present results provided sensitive and useful method for the determination of verbenone 10-hydroxylation catalyzed by rat liver microsomes.

P-57

Ultra-Fast GC for the Determination of Essential Oil Composition and Adulteration

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Capillary GC is applied in different areas such as process control, biology, medicine, pharmacy, environmental control, food and beverages, etc. For the analysis of these complex samples long columns (30 m or more) are used to obtain an high number of plates.
As a consequence, analysis time is very long. Narrowbore columns allow fast separation as proven by the Golay equation. Maintaining the phase ratio β very high the contribute of resistance to mass transfer in the liquid phase to band broadening is very small, and can be neglected. In this case the minimum plate height at the optimum linear velocity will approach the value of the column diameter.
These parameters for the selection of experimental conditions were optimized for the analysis of citrus essential oils.
This approach permits the separation of the components of the volatile fraction of lemon, bergamot, mandarin, lime, sweet orange and bitter orange oils in about 9 minutes, maintaining the same resolution as a conventional GC analysis of about 50 minutes, and with quantitative results that well agree each other. In addition, fast GC/MS coupling permits to acquire MS spectra free from interference, easier to compare with those of standard components, since capillary columns used for fast GC analysis give a very low bleeding due to the very thin film of stationary phase.

P-58

Chemical composition of the Essential oil of *Chaerophyllum macropodum* Boiss. from Iran

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Hydro-distilled volatile oil from the aerial parts of *Chaerophyllum macrospodum* Boiss. (Umbelliferae) was obtained at yield of 0.9% w/w based on dry weight. The oil was analyzed by a combination of GC and GC/MS. 19 compounds were identfied in the oil, representing approximately 99% of the oil. The main constituents of the essential oil were (E)-ß-ocimene (41%), γ-terpinene (35.9%), *p*-cymene (6.5%) and linalool (5.1%). The other compounds present in apreciable amounts are (*Z*)-ß-ocimene (3.5%), fenchyl acetate (1.8%) and terpinolene (1.14%).

References

1. Adams, RP. *Identification of Essential Oils by Ion Trap Mass Spectroscopy.* Academic Press: San Diego, CA, 1989.
2. Mozaffarian V. *The Family of Umbelliferae in Iran.* Research Institute of Forest and Rangelands, no.35, 1983.
3. Sandra P, Bicchi C. *Capillary Gas Chromatography in Essential Oil Analysis,* Alfred Huethig Verlag: New York, 1987 .
4. Mozaffarian V. *A Dictionary of Iranian Plant names,* Farhang Moaser, Tehran, p 407 , 1996.

P-59

How an antibiotic affects essential oil formation

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The antibiotic tetracycline inhibits protein synthesis on the 70S ribosome by binding to its 30S-subunit. Therefore it became a valuable tool in plant physiology to determine the location of physiological processes within a cell, because it only affects processes in plastids or mitochondria. Obviously, tetracycline is influencing the photosynthesis apparatus.
Tetracycline was applied to three genotypes of marjoram (*Origanum majorana* L.) to study its influence on essential oil formation. Two of the genotypes showed a significantly lower number of essential oil glands, while the third genotype was totally unaffected. The density of oil glands was in direct correlation to the content of chlorophyll B. This would allow a cautious hypothesis that essential oil gland formation may be linked to photosynthesis. The pattern of essential oil composition was affected too, especially the formation of *cis*-sabinene hydrate acetate. The portion of sesquiterpenes in the essential oil was augmented as could be expected due to the different cell compartments where the synthesis of mono- and sesquiterpenes, takes place.

P-60

Changes in content and chemical composition of *Pimpinella anisum* oil at various harvest time

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Anise (*Pimpinella anisum* L.) is an annual, herbaceous essential oil plant belonging to the Apiaceae family. It is native to the eastern coast area of Mediterranean to Asia Minor region. The essential oil extracted from *Pimpinella anisum* fruit has antiseptic, antispasmodic, carminative, digestive and fungicide effects. It is also used in perfumes, toothpaste and the liquor industry .The essential oil content and chemical composition of *Pimpinella anisum* fruit was determined at different harvesting times of waxy (with 26 to 28% moisture) and ripening stages. The essential oil was obtained by hydro distillation of fruits, and was analyzed by GC and GC/MS. The oil content of fruits harvested at waxy (unripe) and ripe stages were 5.5 % and 3.4 % respectively. Eight and eleven components have been identified in the oils of waxy and ripe fruits respectively. The major components of the oil of waxy stage were *trans*-anethole (90.35%), estragole (3.6%), eugenyl acetate (3.34%) and the main components of the oil of ripe fruit were, *trans*-anethole (80.7%), eugenyl acetate (3.92%), γ-himachalene (3.52%), estragole (2.27%) and α-zingiberene (1.9%).

P-61

Essential oil composition from the different parts of *Eryngium bourgatti* Gouan from Spain

Jesús Palá-Paúl[a], Mª José Pérez-Alonso [a], Arturo Velasco-Negueruela[a], Jesús Sanz[b], Joseph J. Brophy[c]

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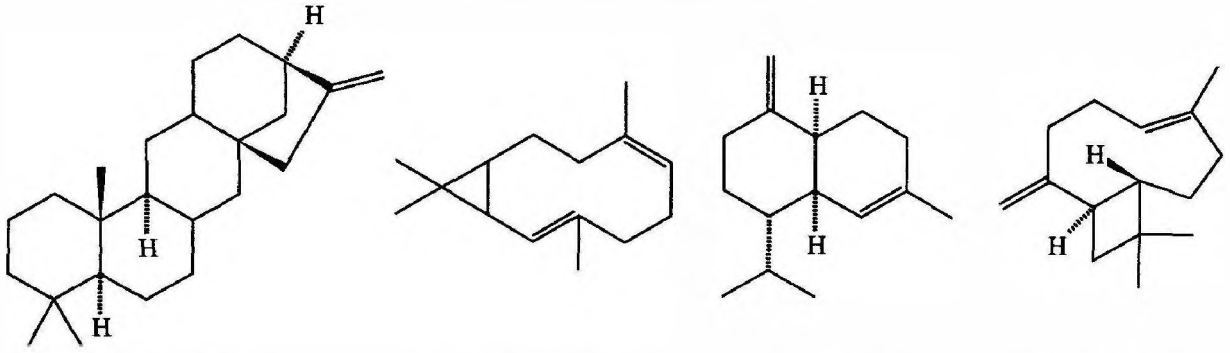
The *Eryngium* L. genus belongs to the Apiaceae family and, with about 250 species, has a cosmopolitan distribution. In the Iberian Peninsula grow 14 of the 26 species described in Flora Europaea. Although *Eryngium bourgatii* Gouan. grows wildly in Spain and France, has been used as an ornamental plant in other countries because of the colour of its leaves and inflorescences.

The essential oil form the different parts of *E. bourgatii* L., stems + leaves, inflorescences and roots, have been extracted by steam distillation and analysed by Gas Chromatography (GC) and Gas Chromatography coupled to Mass Spectrometry (GC-MS). Quantitative but not qualitative differences have been found between the analysed parts. The principal compounds from the inflorescences oil were found to be phyllocladene (37.6%) and bicyclogermacrene (15.1%), while the oil from stems and leaves showed phyllocladene (20.4%), γ-muurolene (11.8%) and (*E*)-caryophyllene (10.1%) as main one. The oil from the roots presented γ-muurolene (15.4%) and phyllocladene (15.0%) as major constituents. It is worth mentioning the presence of a diterpene, phyllocladene, as main compound of the essential oil.

Main constituents



phyllocladene bicyclogermacrene γ-muurolene (*E*)-caryophyllene

P-62

Essential oil composition of two variants of *Prostanthera lasianthos* Labill. from Australia

Jesús Palá-Paúl[a], Lachlan M. Copeland[b], Joseph J. Brophy[c], Robert J. Goldsack[c].
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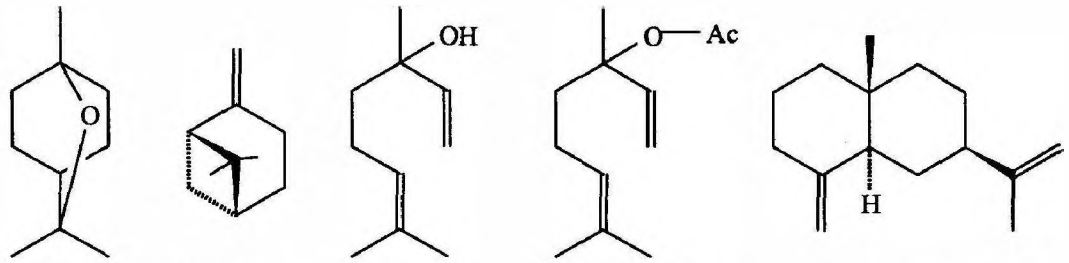
[c]School of Chemistry, The University of New South Wales, Sydney NSW-2052, Australia

The mint family, or Lamiaceae, is famous for the many plants which produce so many of the flavouring substances and culinary herbs in use throughout the ages. The genus *Prostanthera*, belonging to this family, consists of around 100 species that are endemic to Australia. Two variants of *Prostanthera lasianthos* Labill., commonly named "Victorian Christmas Bush", have been previously described as *Prostanthera lasianthos* Rheophytic variant (P.l.R.) and *Prostanthera lasianthos* New England smooth-leaved variant (P.l..N.E.) (1).

Although the species of *Prostanthera* are collectively known as "mint bushes" and are generally reported to have aromatic foliage (2), we could not find any previous study about the chemical composition of *Prostanthera lasianthos*. The essential oils from the aerial parts of three individuals of both the forms have been analysed by GC and GC/MS.

The chemical composition of both samples showed qualitative and quantitative differences. The P.l.R. variant had 1,8-cineole (66.0%-57.3%) and β-pinene (10.2%-8.74%) as principal compounds with a percentage composition higher than 70% of the total oil. The main constituents from the essential oil extracted from P.l..N.E. were found to be linalool (13.8%-9.9%), linalyl acetate (13.8%-7.3%) and β-selinene (12.6%-7.8%). The morphologicaly differences of both variants are also exhibited in their essential oils so there is further evidence to suggest that they should be recognised as distinct taxa at the species level.

Main constituents



1,8-cineole β-pinene Linalool Linalyl acetate β-selinene

1. B. J. Conn. 1992. Flora of New South Wales, Vol. 3. (Ed. G. Harden) Kensington NSW: NSW University Press.
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P-61

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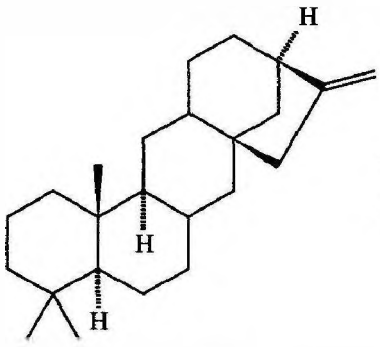
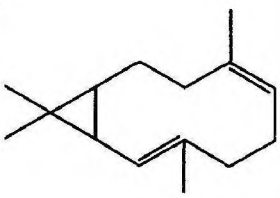
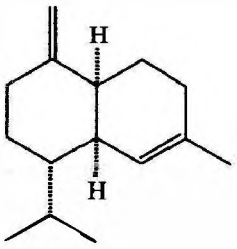
Main constituents



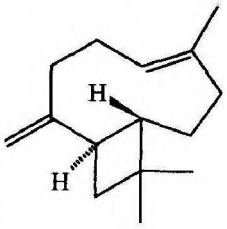
phyllocladene



bicyclogermacrene



γ-muurolene



(*E*)-caryophyllene

P-62

Essential oil composition of two variants of *Prostanthera lasianthos* Labill. from Australia

Jesús Palá-Paúl[a], Lachlan M. Copeland[b], Joseph J. Brophy[c], Robert J. Goldsack[c].
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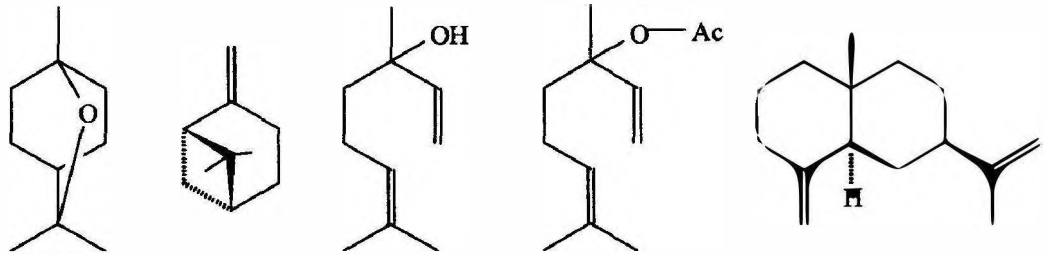
The chemical composition of both samples showed qualitative and quantitative differences. The P.l.R. variant had 1,8-cineole (66.0%-57.3%) and β-pinene (10.2%-8.74%) as principal compounds with a percentage composition higher than 70% of the total oil. The main constituents from the essential oil extracted from P.l..N.E. were found to be linalool (13.8%-9.9%), linalyl acetate (13.8%-7.3%) and β-selinene (12.6%-7.8%). The morphologicaly differences of both variants are also exhibited in their essential oils so there is further evidence to suggest that they should be recognised as distinct taxa at the species level.

Main constituents



1,8-cineole β-pinene Linalool Linalyl acetate β-selinene

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P-63

The essential oil of *Micromeria juliana*: composition and antimicrobial activity

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Species of genus *Micromeria* are restricted spreading to the East and South Europe and Balkan Peninsula. To the best of our knowledge there is only one reference concerning the composition of the essential oil[i] and one about antimicrobial activity[ii]. The aim of this paper is to present the chemical composition and antimicrobial activity of *M. juliana* essential oil.

The essential oil was obtained from the ground and dried aerial parts of *M. juliana* by standard procedure. This yielded in 0.1% of yellow oil with pleasant odour calculated per weight of dry plant material (w/w). The *GC/MS* analysis showed that the main compounds of the oil were verbenol (11.8%), caryophyllene oxide (10.5%), borneol (9.3%) and myrtenal (7.1%).

The antimicrobial activity was tested by disk diffusion method, against following six microorganisms: *Escherichia coli* 95, *Staphylococcus aureus* 6538 ATCC, *Pseudomonas aeruginosa, Klebsiella pneumoniae, Salmonella enteritidis* and *Aspergillus niger*.

In a dilution of 1:20 the oil showed activity only against *Staphylococcus aureus*.

P-64

The essential oil of *Micromeria kosaninii*: composition and antimicrobial activity

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To the best of our knowledge there are no reports concerning composition and antimicrobial activity of *Micromeria kosaninii* essential oil. Therefore we decided to investigate this subject.

The essential oil was obtained from the ground and dried aerial parts of *M. kosaninii* by standard procedure. This yielded in 0.1% of yellow oil with pleasant odour calculated per weight of dry plant material (w/w). The GC/MS analysis showed that the main compounds of the oil were caryophyllene oxide (18.8%), caryophyllene (6.9%) and borneol (6.2%).

The antimicrobial activity was tested by disk diffusion method, against following six microorganisms: *Escherichia coli*, *Staphylococcus aureus*, *Pseudomonas aeruginosa, Klebsiella pneumoniae, Salmonella enteritidis* and *Aspergillus niger*.

The ethanol oil solution in 1 : 20 dilution (4.6 μl of the pure essential oil per disk) showed antimicrobial activity against all microorganisms except against *Salmonella enteritidis*.

P-65

Variation of the yield and carvacrol content of the essential oil in a collection of summer savory (*Satureja hortensis* L.)

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Essential oils of different *Lamiaceae* (*Origanum*, *Thymus*) are increasingly used because of their antimicrobial and antioxidative effects. The aim of the investigations was to prove the suitability of 34 different summer savory populations for the production of carvacrol rich essentail oil. The cultivars and accessions were kindly provided by companies, botanical gardens and gene banks. Thirty plants of each population were planted in summer 2001 and harvested in autumn individually in the flowering stage and dried under natural conditions. The yield of the leaf-flower-fraction was determined by separating it from the stems manually, the essential oil content of the leaves (% v/w) by hydrodistillation, and the carvacrol content of the essential oil by gas chromatography. The mean of the populations average leaf-flower-fraction yield per individual plant was 9.5 g ranging from 4.5 to 17.8 g, the mean of the essential oil content was 2.33% ranging from 1.25% to 3.50%, and the mean of the carvacrol content was 65.2% ranging from 54.2% to 88.3%. Taking account of the leaf yield and the essential oil content, the mean of the essential oil yield of the individual plants was calculated with 0.206 ml ranging from 0.053 to 0.368 ml. The great variability among the populations provides good prerequisites for breeding high performance cultivars by combining aspired chemical and agronomical characteristics which are scattered at present among different populations of the savory collection.

P-66

Larvicidal and Repellancy Effect of Essential oil of *Cymbopogon winterianus* Against Mosquitoes and Isolation of its Bioactive Compopunds

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Cymbopogon winterianus is an aromatic grass which is being extensively used as insect repellent traditionally in the North Eastern part of India and many other parts of the globe. To have a scientific validation of the utility of this plant against mosquitoes the present study was carried out against *Aedes aegypti* and *Culex quinquefasciatus.* The essential oil was extracted with the help of Clevenger apparatus and the relative bioefficacy was studied at the concentration of 10 ppm, 25 ppm, 50 ppm and 100 ppm and observations were recorded at 1hr, 6hrs, 12hrs, 24hrs, 48hrs and 72hrs interval. The lethal concentration (LC_{50}) was calculated after 24 hrs of time interval and was found at 46.88 ppm against *A. aegypti* and 13.27 ppm against *C. quinqufasciatus* . The oil exhibited 80% repellent activity over 3hrs and 30% activity over 4hrs against *C. quinquefasciatus* and 70% and 25% repellent activity respectively over 3hrs and 4hrs against *A. aegypti.* The GC/MS analysis of the oil depicted 59 compounds with citronellal constituting 26.51%, citronellol 11.38% and geraniol 2.27% being the major ones.

The oil was further fractionated into six fractions following fractional distillation under reduced pressure with the help of Cleisen apparatus and by measuring vapour temperature six fractions were collected. These six fractions (F I-VI) were again subjected to bioassay against both the target mosquito species of which FV showed the highest toxicity with LC_{50} value of 12ppm followed by FII with LC_{50} value of 13.4 ppm against *A. aegypti* . Against *C. quinquefasciatus* FII showed the highest toxicity with LC_{50} value of 10.10 ppm followed by that of FV with 14.03 ppm. FI too showed some promise with LC_{50} value of 24.31 ppm. When subjected to repellent test the fraction FI exhibited potency with 60% activity over 4 hrs against *A.aegypti* and 55% in case of *C. quinquefasciatus* .Other fractions did not show any significant results.

These fractions were subjected to GC analysis for identification of the compounds by taking their standard retention time. They were identified as geraniol (FV), limonene (FII) and citronellal (FI).

Allethrin and DEET was taken as control for larvicidal and repellent activity respectively.

P-67

Composition of the essential oils of *Ruta graveolens* L. (Rutaceae) from Peru

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Ruta geaveolens L. (common name Ruda, Rue) is a small evergreen subshrup or semiwoody perennial 2-3' tal and almost as wide. Common ruda is native to southern Europe and northern Africa. It is apparently no longer found in the wild, but occasionally escape from gardens and naturalizes along roadsides and waste areas in North America and Europe, especially in the Balkans.
Ruda's fragrance is strong, characteristically aromatic and sweet; it cannot be compared with any other spice. The waste is rather bitter, even more so when dried. Ruda fruits taste similar, but stronger and somewhat hot. Ruda is mentioned as culinary herb in the New Testament and was a very common spice in ancient Rome, on the other side, its bitterness was proverbial. During the last 2000 years, the ambivalent position gave way to an almost rejection in our days. Like many other bitter spiece, ruda is popular for flavoring liquors.
Ruda contains max 1% of an essential oil, whose main components are 2-undecanone and 2-nonanone plus several more ketones and corresponding secondary alcohols.
The essential oil of Ruda was analyzed on two fused capillary columns with bonded phases of different polarity. Compounds were identified using both chromatographic (RI) and mass spectroscopic criteria. Identities of compounds were establish by use of on-line Wiley 275/NBS75k/NIST mass spectral data bases and literature MS data.
The main components, representing up to 97% of total oil were: 2-undecanone (49%) and 2-nonanone(38%) and 2-decanone (2.5%).

References

Jorge A, Aristides R, Victor F, (1997) *J. Essent. Oil Res.* 9, 365-366
Aboudab E, Elazzouny A, (1998), *Sci. Pharm* 56, 121-124
Yaacob G, Abdullah M, Joulain D, (1989) *J. Essent. Oil. Res* 1, 203-207
Adams R (1995) *Identification of Essential Oil Components by Gas Chromatography/ Mass Spectroscopy.* Allured Pub. Co., Carol Stream, Illinois, USA

P-68

Sesquiterpene constituents in *Mylia taylorii* and *Mylia nuda* (Hepaticae)

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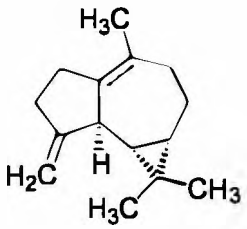
The essential oils of *Mylia taylorii* and *Mylia nuda* (Jungermanniaceae) were investigated by GC and GC / MS and found to exhibit comparable sesquiterpenoid patterns. Many known compounds could be identified by comparison of their mass spectra and retention indices with authentic samples. Several unknown hydrocarbons with the molecular mass $m/z = 202$ (**1** - **5**) and some oxygenated sesquiterpenoids (**6** - **10**), including two novel carbon skeletons (**6** and **7**), were detected and selected for isolation. Their structures were identified by one- and two-dimensional NMR spectroscopy, absolute configurations were determined by chemical correlations and enantioselective gaschromatography.



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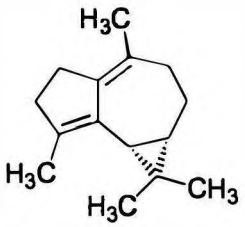

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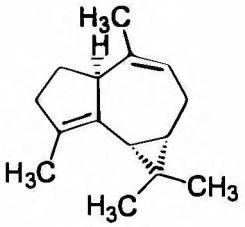

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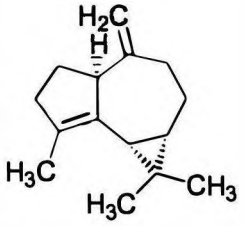

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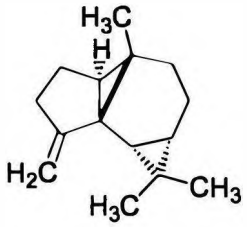

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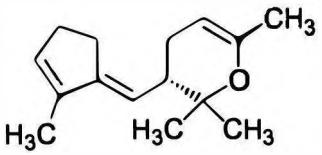

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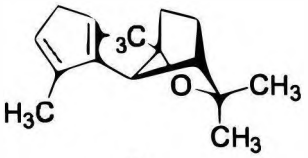

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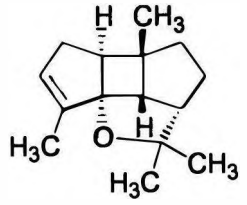

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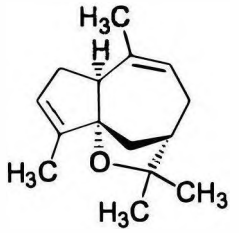

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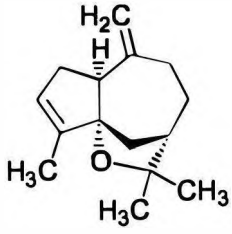

10

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Essential Oils Composition of *Zhumeria majdae* Rech. from three locations in the South of Iran

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Zhumeria majdae Rech. was collected from three main growing places of the plant which are located in the North of Bandar Abbas (the center of Hormozgan, Southern province of Iran) at folwering stage in April 2002. Essential oils were produced by hydrodistillation of dry leaves at the yields of 6.5%, 4.1% and 5.3% (based on dry weights), respectively.GC and GC/MS analyses showed the presence of linalool (55.1%, 60.4% and 59%) and camphor (26.2%, 26.5% and 23.7%) as the two major compounds and some other minor constituents.

P-70

Chemotypical variation of tansy (*Tanacetum vulgare* L.) from 40 different locations of Norway

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Between 2000-2002, plant collections of Norwegian tansy (*Tanacetum vulgare* L.) have been studied with focus on essential oil (EO) yield and variability related to morphological and ontogenetical differences (*b*). Tansy EO is known for infraspecific variability as reported for other aromatic plants (*g*), and chemotypes from different countries have been reported (*a,d,e,f*). Aim of the presented study was to characterize the EO variability of Norwegian tansy from 40 geographical locations (*c*). Tansy collections were transplanted to the Apelsvoll Research Centre Div. Kise in 2000 and grown for two years before harvesting the aerial parts (leaf, stem, flower bud) in June 2002. EO was isolated from dried plant material by hydrodistillation and analysed by GC-MS on a DB5 column at the Plant Biocentre.
The EO yield ranged between 0.35 to 1.90 % (v/w) (average: 0.81 %), and the most abundant thujone-chemotype plants were especially rich in EO volatiles (0.95 %). Based on the GC-MS data, six chemotypes could be identified: thujone (24 individuals), camphor (6(5)), artemisia ketone/ alcohol (3), umbellulone (3), chrysanthenyl acetate/ alcohol (3) and 1,8-cineole (1(2)). The thujone-chemotype was dominated by ß-thujone (81 %) accompanied by traces of α-thujone, but tansy plants rich in α-thujone could also be detected (61 %).

References

(a) Collin, G.J., Deslauriers, H., Pageau, N. and Gagnon, M. 1993. Essential oil of tansy (*Tanacetum vulgare* L.) of Canadian origin. *J.Essential Oil Res.* 5(6):629-638.
(b) Dragland, S., Mordal R. and Rohloff, J. 2003. Tansy (*Tanacetum vulgare* L.): Plant growth, essential oil content and quality of 5 genotypes. *Grønn Forskning* [subm. summer 2003; Norwegian].
(c) Dragland, S., Rohloff, J. and Mordal, R. 2003. Chemotypical variation of tansy (*Tanacetum vulgare* L.) from Norway. *J.Agric. Food Chem.* [subm. summer 2003].
(d) Hendriks, H., van der Elst, D.J.D., van Putten, F.M.S. and Bos, R. 1990. The essential oil of Dutch tansy (*Tanacetum vulgare* L.). *J. Essent. Oil Res.* 2:155-162.
(e) Héthelyi, E., Koczka, I. and Tétényi, P.1989. Phytochemical and antimicrobial analysis of essential oils. *Herba Hung.* 28, (1-2):99.
(f) Keskitalo, M., Pehu, E. & J. E. Simon 2001. Variation in volatile compounds from tansy (*Tanacetum vulgare* L.) related to genetic and morphological differences of genotypes. *Biochem.Syst.Ecol.* 29:267-285.
(g) Rohloff, J. 2003. Essential Oil Drugs - Terpene Composition of Aromatic Herbs, *In* Production Practices and Quality Assessment of Food Crops. Vol. 4: Post Harvest Treatments. Ed. Dris, R., Kluwer Academic Publishers, Dordrecht, 59p. [publ. 2003].

P-71

Volatile Constituents of *Ballota aucheri* Boiss., *Stachys benthamiana* Boiss. and *Perovskia abrotanoides* Karel. three Labiatae Herbs Growing Wild in Iran

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The genus *Ballota* consists of about 33 species growing mainly in the Mediterranean region. In Iran the genus *Ballota* is represented by three species: *B. aucheri* Boiss., *B. nigra* L. and *B. platyloma* Rech. f. , of which *B. aucheri* and *B. platyloma* are endemic plants (1). Some species are used in folk medicine, the leaves and the tops of *B. saxatilis* are used for colic, asthma, influenza, in somnia and hemorrhoids. The infusions prepared from the leaves are reported to possess antiulcer, antispasmodic, and sedative activities. The genus *Stachys*, consists of about 200 species wide spread throughout the world. In Iran 34 species are present, among which 13 are endemic (1). The *Perovskia* genus is presented in Iran by three species: *P. abrotanoides*, Karel., *P. artemisoides* Boiss. and *P. artiplicifolia* Benth.(1).

The composition of the essential oils from three Labiatae species of Iran: *Ballota aucheri* Boiss., *Stachys benthamiana* Boiss., which are endemic to Iran, and *Perovskia abrotanoides* Karel. obtained by hydrodistillation were analyzed by GC and GC/MS. α-Cadinol (21.0%) and dehydroaromadendrane (11.8%) were the main components among the thirty-seven constituents characterized in the oil of *Ballota aucheri* representing 82.5% of the total components detected. Twenty compounds were identified in the oil of *Stachys benthamiana* representing 91.2% of the total oil with germacrene D (16.8%), linalool (16.6%) and ß-caryophyllene (11.0%) as the major constituents. The oil of *Perovskia abrotanoides* was characterized by higher amount of 1,8-cineole (28.0%) and camphor (24.0%) among the twenty-three components comprising 84.3% of the total oil detected. The oils (*Ballota aucheri* and *Stachys benthamiana*) consisted mainly of sesquiterpenes, while in *Perovskia abrotanoides* oil monoterpenes predominated over sesquiterpenes.

1. K. H. Rechinger, *Ballota, Stachys* and *Perovskia* in: *Flora Iranica*, Labiatae No. 150. Edits.,
K. H. Rechinger and I. C.Hedge, pp. 350, 370, Akademische Druck and Verlagsanstalt, Graz, Austria (1982).

P-72

Chemical composition and antifungal activity of the essential oil of *Thymbra capitata* on *Candida*, *Aspergillus* and Dermatophyte species

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The composition and the antifungal activity of the essential oil of *Thymbra capitata* on *Candida*, *Aspergillus* and dermatophyte strains were studied in order to support its use as antifungal agent. The composition of the essential oils of twenty-two populations of *T. capitata* from Portugal (Algarve and Estremadura) was investigated by GC and GC-MS. The oils from all samples are carvacrol type, with high content of carvacrol (60.0-65.8%) and its biogenetic precursors, γ-terpinene (8.2-9.5%) and *p*-cymene (6.0-7.5%).
Thymol and thymol/carvacrol chemotypes were not found in Portugal.
The minimal inhibitory concentration (MIC) determined according to the NCCLS protocols (M27-A and M38-P) and the minimal lethal concentration (MLC) were used to evaluate the antifungal activity against *Candida* (7 clinical isolates and 3 ATCC type strains), *Aspergillus* strains (5 clinical isolates, 2 ATCC and 2 CECT strains) and dermatophyte clinical strains (*Microsporum canis*, *M. gypseum*, *Trichophyton rubrum*, *T. mentagrophytes*, *Epidermophyton floccosum*). The oil exhibited significant antifungal activity for the most of the tested strains. MIC and MLC values are similar for *Aspergillus* and *Candida* strains, ranging from 0.16 to 0.32 µl/ml. For dermatophytes MIC and MLC values are similar for all the strains, ranging from 0.08 to 0.32 µl/ml. The antifungal activity of the major compounds (carvacrol, γ-terpinene and *p*-cymene) was also evaluated allowing to conclude that they can be responsible for the oil activity.

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P-73

In vivo mapping of essential oil plants by micro Raman spectroscopy

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Several attempts have been made during the last years to use various vibrational spectroscopy methods for quantification of valuable components in essential oil plants as well as rapid discrimination of different chemotypes [1-4]. Whereas interpretation of NIR spectroscopic results is only possible on the basis of suitable reference data (e.g. physical-chemical parameters, GC analysis data) applying various chemometric algorithms, Raman spectroscopy principally allows to identify non-destructively characteristic key bands of distinctive essential oil substances in the fresh plant. Using Nd:YAG (neodymium doped yttrium aluminium garnet) laser excitation at 1064 nm thermal decomposition of the object as well as strong fluorescence can be avoided. Using a Fourier-Transform Raman spectrometer coupled with a microscope it is also possible to map in vivo the distribution pattern of secondary substances directly in the essential oil glands. Relating to characteristic key bands a reliable discrimination of different chemotypes within the same species can be successfully performed. Furthermore, the special advantage of Raman mapping is that time and/or location induced changes (e.g. biochemical processes caused by stress phenomena or insect attack) can be detected in the living plant.

1. Schulz H, HH Drews, H Krüger (1999) Rapid NIRS determination of quality parameters in leaves and isolated essential oils of Mentha species, *J. Essent. Oil Res.* **11**, 185-190.
2. Steuer B, H Schulz, E Läger (2001) Classification and analysis of citrus oils by NIR spectroscopy, *Food Chemistry* **72**, 113-117.
3. Schulz H, B Schrader, R Quilitzsch, S Pfeffer, H Krüger (2003) Rapid classification of basil chemotypes by various vibrational spectroscopy methods. *J. Agric. Food Chem.* **51**, 2475-2481.
4. Schulz H (2003) Rapid evaluation and quantitative analysis of thyme, origano and chamomile essential oils by ATR-IR and NIR spectroscopy, *J. Mol. Struct.* (in press).

P-74

Chemical variation in the essential oil of *Satureja sahandica* from Iran

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Hydro-distilled volatile oils from the aerial parts of eight populations of *Satureja sahandica* Bornm. were investigated mainly by a combination of GC and GC/MS. *S. sahandica* is one of the endemic species of *Satureja* in Iran. Thirty-nine components were identified in the oils. The main constituents of the essential oils were thymol (19.6%-41.7%), p-cymene (32.5%-54.9%) and γ-terpinene (1.0%-12.8%). Although the main components of all the oils are common, but the percentage of them are different. There are some minor components in some of the oils that are not present in the other.

P-75

Online determination of $^{2}H/^{1}H$ and $^{13}C/^{12}C$ isotope ratios of cinnamaldehyde from different sources using gas chromatography isotope ratio mass spectrometry

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The combination of gas chromatography-combustion-isotope ratio mass spectrometry (GC-C-IRMS) and gas chromatography-pyrolysis-isotope ratio mass spectrometry (GC-P-IRMS) is applied to the authenticity assessment of cinnamaldehyde from various sources. Adulterations of ceylon bark oil with cinnamon oils of minor quality are attractive due to the more subtle and aromatic ceylon bark oil is most expensive. For that reason, from three different varieties of cinnamon bark on the market, *C. ceylanicum* (ceylon) mostly grown in Sri Lanka, *C. cassia* (cassia) known as chinese cinnamon and *C. burmanii* (cassia vera) mostly grown in Indonesia, cinnamon oils were self-prepared by steam-distillation. Furthermore, the so-called wood cinnamon was investigated, which is made of the outer bark of older branches of cinnamon of minor quality. From commercial cinnamon powder self-prepared oils were analysed. In addition several commercial samples of cinnamon oil and cinnamaldehyde, some of them declared to be natural, were investigated.
$\delta^{2}H_{V\text{-}SMOW}$ and $\delta^{13}C_{V\text{-}PDB}$ values of cinnamaldehyde were determined and characteristic authenticity ranges were deduced, allowing the differentiation between synthetic and natural samples. By correlation of both the $\delta^{2}H_{V\text{-}SMOW}$ and $\delta^{13}C_{V\text{-}PDB}$ values, characteristic authenticity ranges could be defined for the more important varieties of cinnamon ceylon and cassia. By comparing the $\delta^{2}H_{V\text{-}SMOW}$ values of different self-prepared samples (ground bark, distillate) of cinnamon determined by TC/EA-IRMS with the corresponding GC-IRMS values, online GC-IRMS methods are proved to be essential in the authentication of complex natural products.

References

[1] Senanayake UM, Terence LH, Wills RBH (1978) J. Agric. Food Chem. 26:822-824
[2] Bilke S, Mosandl A (2002) Rapid Commun. Mass Spectrom. 16:468-472
[3] Culp A, Noakes JE (1990) J. Agric. Food Chem. 38:1249-1255
[4] Roth Kormann (1997) Duftpflanzen Pflanzendüfte, ecomed pp100ff, 272f, 478
[5] H.B.Heath (1981) Source Book of Flavors, The Avi Publishing Company, Inc. Westport, pp233 –236
[6] Gassner, Hohmann, Deutschmann (1989) Mikroskopische Untersuchung pflanzlicher Lebensmittel, 5th Edition, Gustav Fischer Verlag Stuttgart, Germany, pp 335-344
[7] Sewenig S, Hener U, Mosandl A (2003) Eur Food Res Technol, in press

P-76

The Blue Essential Oils of some Plants from Eastern Mongolia and Desert-Gobi

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The blue essential oils of some aromatic plant species are important with regard to cosmetic and aromotherapeutic aspects. The blue essential oils were produced by steam distillation and analyzed by GC and GC/MS.

Guaiazulene was present in the essential oils of *Ajania achilleoides* Poljak, *Artemisia macrocephala*, *Artemisia frigida* Willd, *Artemisia rutifolia* Steph, *Artemisia gmelinii* Stechm, *Artemisia sericea*, *Chtysanthemum zawadskii* and *Heteropappus altaica.*

In addition, a blue essential oil was pbtained from *Brachanthemum mongolorum* Grub consisting of 72 compounds including ß-caryophyllene (12.77%), guaiazulene (11.72%), germacrene-D (11.01%), 1.8-cineole (5.52%) and camphor (4.37%), which had the highest percentages.

The leaves of *Brachanthemum gobicum* Krasch, which were collected from two different locations (Middle Gobi and Southern Gobi), had 34 compounds. The major constituents were 1.8-cineole (32-44%), camphor (28.48%) and guaiol (12.35%). During the steam distillation guaiol (12.35-31.58%) was obtained.

The essential oil of *Ferula ferulaodes* Korov had 37 compounds including guaiol (58.76%) nerolidol (10.21%), α-eudesmol (3.05%), ß-farnesene (3.02%), dihydroeudesmol (2.01%), which were the major constituents.

Natural origins of chamazulene:

The essential oil from dry leaves and seeds of *Artemisia Sieversiana* Willd prepared in the winter had 7 compounds. The major constituents were myrcene (26.56%), 1.8-ceneole (11.94%), chamazulene (10.26%), linalool (8.36%, borneol (6.40%) and p-cymene (5.39%).

Essential oil from dry leaves and flowers of *Artemisia mongolica* had 73 compounds. The major constituents of the essential oil were 1.8-cineole (14.58%), cis-ocimene (14.61%), germacrene d (11.30%), camphor (7.10%), β-thujone (5.37%), cis-chrysanthenol (4.44%), myrcene (4.26%), α-selinene (3.36%), and sabinene (2.23%).

In the essential oil of *Achillea ptarmicoides* 38 compounds were identified. The major constituents were chamazulene (32.92%), germacrene-D (11.00%), caryophyllene (7.39%), 1.8-cineole (6.45%), camphor (4.10%), caryophyllene oxide (3.24%) and guaiol (2.12%).

Moreover, in the essential oil of an other species of this genus (*A. asiatica*) 38 compounds were identified. The major constituents of the essential oil were 1.8-cineole (11.7%), chamazulene (9.85%), ß-caryophyllene (8.00%), α-terpineol (6.20%), germacrene-D (4.62%), and camphor (2.52%).

P-77

Taxonomic analysis of Portuguese *Thymus* species using AFLP (Amplified Fragment Length Polymorphism) markers

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The genus *Thymus* is a very wide and taxonomically complex group of *Labiatae* aromatic plants. Aiming to contribute for the taxonomy of this genus, Amplified Fragment Length Polymorphism (AFLP) analysis was used to clarify the genetic relationships among 7 *Thymus* species growing in Portugal: *T. mastichina* (L.) L. subsp. *mastichina*, *T. albicans* Hoffmanns. & Link, *T. lotocephalus* G. López & R. Morales, *T. villosus* L. subsp. *villosus*, *T. camphoratus* Hoffmanns. & Link *T. carnosus* Boiss and *T. capitellatus* Hoffmanns. & Link, Samples of 44 populations of the 7 thyme species were collected from January to March 2002 in the Portuguese regions of Algarve, Baixo-Alentejo, Alto-Alentejo and Estremadura. Cuttings were taken from each plant and rooted in pots, forming a collection presently maintained at the University of Algarve.
Modifications were introduced to the DNA extraction protocol routinely used in the Laboratory of Genetics and Plant Breeding, in order that high quality thyme genomic DNA could be extracted. AFLP analyses were performed successfully and characteristic molecular patterns were generated for each population. Using the NTSYs program, the UPGMA algorithm and based on the AFLP markers, a genetic similarity dendrogram was constructed. Proving their tighter genetic similarity, populations within each species formed clusters obviously discernable from clusters among species. Genetic similarity between species, and their respective distribution and branching in the dendrogram, confirmed the taxonomic classification based on phenotypic traits. Correlation was found between genetic similarity among populations within each species and their geographic proximity.

Acknowledgment: D.V. da Silva is the recipient of the Ph.D. fellowship SFRH/BD/4729/2001 from Fundação para a Ciência e a Tecnologia with the support of FSE-IIIQCA

P-78

Genetic and chemical composition analysis of *Thymus mastichina* (L.) L. subsp. *mastichina* from Portugal

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Thymus mastichina is an Iberian Peninsula endemic Labiatae, widespread in Portugal. Regarding the composition of its essential oils, three distinct chemotypes were found in Portugal (1,8-cineole, linalool and 1,8-cineole/linalool) [1]. The aim of this work was to search for correlations between chemical compositions of essential oils and genetic profiles of the plants. For this purpose, 10 populations from different regions of Portugal, 15 individuals each, were collected and genetic profiles of the populations were established using Amplified Fragment Length Polymorphism (AFLP) markers. 1,8-Cineole (39.9-65.1%) is the major component of the essential oils of eight of these populations. The oils of plants from the other two populations (from Estremadura) are predominantly constituted by linalool (63.0%) or by 1,8-cineole and linalool (31.2% and 29.8% respectively).
Nine populations were found genetically similar exhibiting genetic similarity coefficient values over 0.98. Nevertheless, one population from SE Portugal, although characterised by 1,8-cineole chemotype oils, clearly separates apart in the constructed genetic similarity dendrogram.
Genetically indiscernible samples collected in same geographic region exhibited always a similar oil composition. On the other hand, samples from different geographic regions or having different oil composition always appear genetically more distanced in the dendrogram.

Acknowledgment: D. V. da Silva is the recipient of the Ph.D. fellowship SFRH/BD/4729/2001 from Fundação para a Ciência e a Tecnologia with the support of FSE-IIIQCA

[1] Salgueiro, L., *Ph.D. thesis "Os tomilhos portugueses e os seus óleos essenciais"*, vol.1, 1994

P-79

Composition and Antibacterial Activity of *Achillea clypeolata* Essential Oil

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Volatile oil of wild growing population of *Achillea clypeolata* Sibth. et Sm. (*Asteraceae*) was studied for yield, composition and antibacterial activity. Eighteen identified components constituted 89.8% of the oil. The major components in the oil were *(E)*-γ-bisabolene (17.9%), 1,8-cineole (16.0%), borneol (11.9%) and caryophyllene-oxide (11.5%) reaching together 57.3% of the total oil content. *(E)*-γ-bisabolene seems to be not only the most abundant component in the oil, but also the component reported for the first time in the genus. In an antibacterial diffusion assay, the oil showed activity against all tested Gram-negative bacteria (*Escherichia coli, Klebsiella pneumoniae* and *Pseudomonas aeruginosa*) and Gram-positive *Staphylococcus aureus*.

P-80

The essential oil of *Achillea clavennae*: composition and antimicrobial activity

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Different species of the genus *Achillea* L. are widely used in folk medicine because of their numerous beneficial properties.

Probably due to it's restricted spreading to the East and South Alps and west parts of Balkan Peninsula little attention has been given so far to *Achillea clavennae*. To the best of our knowledge there is only one reference[1] concerning the composition of the essential oil and none about its antimicrobial activity. The aim of this paper is to present the chemical composition and antimicrobial activity of *A. clavennae* essential oil.

The essential oil was obtained from the ground and dried aerial parts of *A. clavennae* by standard procedure. This yielded in 0.12% of green oil with pleasant hay odour calculated per weight of dry plant material (w/w). The *GC/MS* analysis showed that the main compounds of the oil were camphor (41.9%) and 1,8-cineole (22.5%) with minor amounts of borneol (7.9%) and á-terpineol (7.4%).

The antibacterial activity of the oil was investigated by disk diffusion method. The following 6 microorganisms were used: *E. coli*, *S. aureus*, *K. pneumoniae*, *P. aeruginosa*, *A. niger* and *C. albicans*.

The ethanol oil solution showed moderate antimicrobial activity even at the dilution of 1:60 to all used stains of bacteria. Both the Gram-positive stained and Gram-negative stained bacteria had approximately equal non-resistance to the oil. However the *A. clavennae* essential oil showed high activity against the pathogen fungi.

Reference:

1. Chalchat, J., Gorunovic, M., Petrovic, S., Zlatkovic, V., *J. Essent. Oil Res.*, 2000, **12** (7-9) 7.

P-81

Antimicrobial activity of *Nepeta rtanjensis* essential oil

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Nepeta rtanjensis was found and established in 1974 and presents an endemic species for Serbia occurring on a few natural localities on the Rtanj mountain. To the best of our knowledge only three references deal with the essential oil composition and none of them deals with the antimicrobial activity of the oil.

The amounts of yellowish highly fragrant oils obtained in a Clevenger type apparatus were 0.8 % and 1.0 % (w/w, growing wild and cultivated, respectively).

The main compound in both samples was 4aα,7α,7aβ-nepetalactone, physologically active towards certaine insects, with 83.6 % (wild) and 77.9 % (cultivated). α-Copaene, germacrene D and δ-cadinene were present in a much lesser extent (less than 5 %) in the oils.

The antimicrobial activity of the oil was investigated by disk diffusion method with Ampicilin as the standard antibiotic. The following 6 microorganisms were used: *E. coli*, *S. aureus*, *K. pneumoniae*, *P. aeruginosa*, *S. enteritidis*, *A. niger*. The activity of the ethanol oil solution in 1 : 10 dilution (4.6 μl of the pure essential oil per disk) was greater than the activity of the standard antibiotic (10 μg of Ampicilin) and in 1 : 30 dilution (1.6 μl of the oil per disk) approximately equal to the antibiotic activity against all the microorganisms. The oil showed bacteriostatic activity even in 1 : 60 dilution. The oil inhibited the growth of fungi but has not showed fungicide activity.

P-82

Chemical Characterization of some Interspecific Hybrids of the Genus *Allium* in Comparison to their Parental Species

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The health value of cultivated species belonging to the genus *Allium* has become more and more a topic of discussion. Several studies have shown widespread field of application such as cancer protective, antibiotic and antiasthmatic properties. Many wild species of the genus *Allium* presenting interesting distributions or amounts of cysteine sulphoxides which are made responsible for the health properties as well as their typical aroma on metabolisation in an enzymatic reaction with alliinase. In most cases the wild plants are small and it is difficult to cultivate them. By applying cross-breeding experiments the chemical properties (aroma- or cysteine sulphoxide pattern) of this species can partially be transferred to cultivated *Allium* plants (e.g. onion or leek) and the resulting hybrids usually show an increased size of the bulbs. The aim of our study was to characterise the hybrids and their parental species on the basis of their sulphur-containing volatile compounds using SPME-HS-GC analysis. Several of these hybrids especially those obtained with *Allium cepa* (onion) have been investigated. Generally, hybridisation was proved by RADP analysis; the individual aroma profiles were compared to the corresponding cysteine sulphoxide pattern determined by HPLC analysis.

P-83

Investigation of variability in essential oil yield and composition of *Myrica gale* collected from the Scottish Highlands over a period of several years

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Myrica gale L. (bog myrtle) is a robust deciduous shrub that thrives in the wet, peaty soils of the Highlands and Islands of Scotland. Its success on such infertile land is due partly to its symbiotic association with a nitrogen-fixing fungus, which, together with organic matter from its leaves, adds nutrients to the soil. The plant has a unique pleasant fragrance produced by essential oil in its leaves and catkins. It has been traditionally used in folk medicine, as insect repellent, for beer production and as a dye. Myrica exhibits a range of morphological forms with some types producing larger leaves, various differences in branching habit and distribution of male, female and/or bisexual flowers. The volatile oil consists of a range of monoterpenes and sesquiterpenes (between 120-180 components), with approximately 15 compounds having concentrations greater than 1% w/v and comprising about 70% of the total oil. Another 20 compounds were present at between 0.1-1% w/v of total oil, and these represented about 10% of total oil. Fresh plant material was collected from 20 different population sites across the Highlands, and 10 important morphological characteristics were recorded on 5 individual plants from each of the 20 populations. A principal component analysis was performed on the data to examine variability among the accessions for all 10 variables simultaneously. All samples were distilled and analysed by GC, and several representative samples were analyzed by GCMS. Essential oil yield varied between 0.05 – 0.4 % (v/dw). There was a large variability in oil composition, however, and the samples were divided into two groups; a group with a high monoterpene fraction (alpha-pinene, limonene, 1,8-cineole, alpha-phellandrene, *p*-cymene), and a group with a high sesquiterpene fraction (caryophyllene, delta-cadinene, germacrene B, nerolidol, elemonene, elemene, copaene). The pattern of variability amongst these main components could not be attributed to any particular factor, including harvest time, position of the plants within the site, or indeed, the situation of each site. Collections were repeated the following year with similar high variability. Cuttings from several clones were used for the successful establishment of shoot tissue culture with the aim of producing a stable clonal population.

SAC received financial support from SEERAD and BBSRC. Thanks to A. Syred for microphotographs of glands and flowers (Microscopix, Wales); to Highland Natural Products for arrangement of collection sites; to CPL Aromas for GCMS.

P-84

Phytochemical Investigation of *Mentha aquatica* Collected From Native Scottish Populations

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Mentha aquatica L. (water mint) is a perennial species, widely distributed throughout Europe and found in the British Islands. It grows in shallow water, on the banks of ponds, streams and ditches and in marshes and wet meadows. The plant flowers from June to September and hybridises easily with other mint species. The most famous hybrid is *M. piperita* which appeared spontaneously and has been known since 1750. Several chemotypes of water mint have been described: beta-caryophyllene, 1,8-cineole, germacrene D, linalol, elemol, menthofuran, viridiflorol. Water mint has been employed since ancient times for culinary and medicinal purposes, especially for treating stomach ailments. *M. aquatica* has not been investigated to its full extent as other *Mentha* species, especially regarding its exact botanical description, the variability between plants and the bioactivity of the essential oils. The main collections from natural populations were carried out mainly in Mediterranean regions, but water mint in Scotland has not been collected and analysed previously. In the current study, collections were made from 14 sites across Scotland and one site was chosen for detailed investigation. This latter site, the Carrick Hills, is situated on the West Coast of Scotland, about 1 mile inland and at 300-500 m above sea level. This area is classed as poor moorland, bracken covered unfertile hills, usually wet and with several streams running through them. Within this one location, 4 distinct sample areas were chosen for collection of mint at various phenological stages. A range of samples were collected for their botanical description, essential oil yield and composition. For the 14 sites, the oil yield ranged from 0.4-1.5% (v/dw), although it is possible that some of the samples are not *M. aquatica*, but could be escaped mixed types from household gardens. Carrick Hills site samples are still being analyzed, with a 0.4% oil yield (v/dw) at the vegetative stage. With regard to oil composition, the sites showed high variability, with menthofurane, caryophyllene, piperitone and several not-yet identified peaks being observed. The Carrick Hills type is of a menthofuran chemotype (about 43% of total oil). Further analysis of all samples is in progress. Using SEM, essential oil glands have been observed and described on the calyx, corolla, leaves and stems. The oil will be also tested for antimicrobial properties and toxicity. Selected material will be used for tissue culture propagation.

SAC received financial support from SEERAD. Thanks to A. Syred for microphotographs of glands (Microscopix, Wales); to CPL Aromas for GCMS.

P-85

Terpenoid Lactones from Linalool: Synthesis and Odour Characteristic

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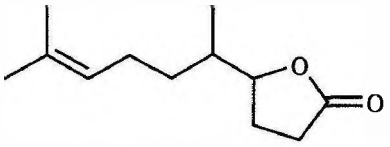
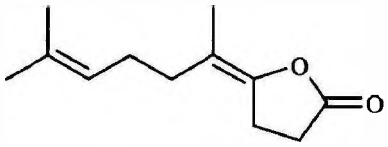
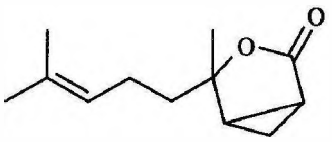
Terpenoid lactones are group of natural compounds possessing specific biological activity like antimicrobial, antifeedant and cytotoxic. Many of them are known as odouriferous substances. We are interested in synthesis of terpenoid lactones as potential insect feeding deterrents and odouriferous substances. Here we present the syntheses of lactones from (±) linalool. Hydrolysis of esters obtained from Claisen rearrangement (ortho-acetate modification) of (±) linalool gave γ-δ unsaturated acids. Reaction of these acids with I_2/KI led to mixture of γand δodolactones. Reduction of mixture of γ-iodolactones with tributyltin hydride (TBTH) led to distereoisomeric mixture of saturated γ-lactones, characterized by fresh–melon odour. Elimination of hydrogen iodide from γ-iodolactones with DBU afforded γ-δ unsaturated γ-lactones **1** and **1c** possessing oryginal mushroom odour. Reaction of δ-iodolactone with DBU gave bicyclic lactone **1d**, with cyclopropane-moiety, having fruity-butter odour. Some of synthesized lactones **1b,c** showed antifeedant activity against *Leptinotarsa decemlineata*.



1a



1b (E) isomer
1c (Z) isomer



1d

P-86

Study on polybasic acid esterification during the ripening fruit

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During fruit (plum, citrus, cherry etc.) ripening, biosynthesis and esterification of polybasic acids (citric acid, malic acid, tartaric acid etc.) occur simultaneously. From the very first stages of ripening, .approx.10 to 50% of polybasic acids in several fruit are totally esterified. During ripening, free polybasic acids decrease in proportion to the rest, while partially esterified polybasic acids increase at the expense of the free fraction and simultaneously a portion of the partially esterified polybasic acids are transformed in totally esterified polybasic acids. In the fully ripe fruit the free carotenoid pigments and the partially and totally esterified forms occur. The esterified polybasic acids are chiefly ethyl-forms, and those ethyl-forms influence the flavour of several fruits.

P-87

A New Phthalide from the Essential Oil of *Meum athamanticum* Jacq.

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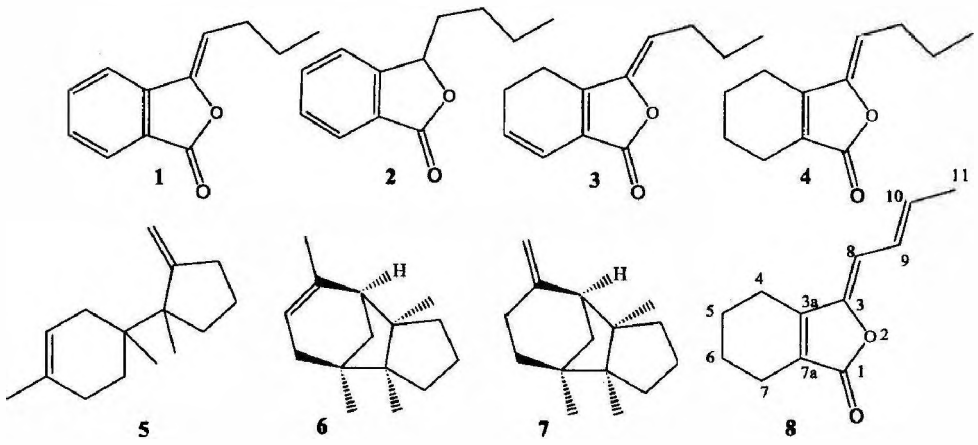
The essential oil of *Meum athamanticum* (L.) Jacq. had previously been investigated several times. Phthalides such as (*Z*)-3-butylidene phthalide (**1**), butylphthalide (**2**), (*Z*)-ligustilide (**3**) and sedanoic acid lactone (**4**) as well as sesquiterpene hydrocarbons such as β-bazzanene (**5**), α- and β-barbatene (**6**, **7**), were reported by Stahl et al., Kubeczka et al. and König et al., respectively. [1-3]. In addition some monoterpene hydrocarbons such as (*E*)-β-ocimene, p-cymene, (*Z*)-β-ocimene, Δ-3-carene were reported as constituents by Kubezka et al. and Tirillini et. al. [3,4].

In this investigation of the leaves of *M. athamanticum*, in addition to several mono- and sesquiterpenes, which were identified by GC-MS, a new phthalide, 3-but-2-enylidene-4,5,6,7-tetrahydro-3H-isobenzofuran-1-one (**8**), together with previously reported (*Z*)-ligustilide (**3**) and sedanoic acid lactone ((*Z*)-butylidene-4,5,6,7-tetrahydrophthalide) (**4**) were isolated and their structures determined by spectroscopic methods.



[1] E. Stahl, H. Bohrmann, *Naturwissenschaften* **1967**, *54*, 118.
[2] W.A. König, A. Rieck, Y. Saritas, I.H. Hardt, K.H. Kubeczka, *Phytochemistry* **1996**,*42*, 461-464.
[3] K.H. Kubeczka, A. Bartsch, I. Ullmann. In: *Essential Oils, Analysis, Physiology, Composition.* K.H. Kubeczka (Edit.), pp 158-187, G. Thieme Verlag Stuttgart, New York (1982).
[4] B. Tirillini, R. Pellegrino, A. Menghini, B. Tomaselli, *J. Essent. Oil Res.* **1999**, *11*, 251-252.

P-88

New Guaiane Type Sesquiterpenes from the Essential Oil of *Peucedanum tauricum* Fruits

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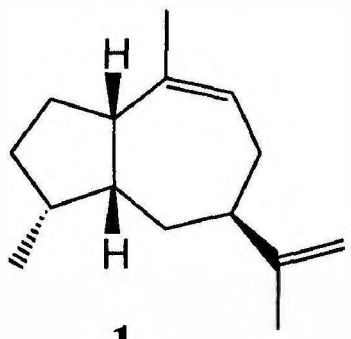
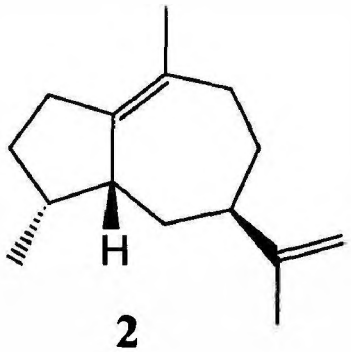
The essential oil of the fruits of *Peucedanum tauricum* (Apiaceae) was investigated using GC, GC-MS and NMR techniques. Several mono- and sesquiterpenes were identified including two new guaiane type sesquiterpene hydrocarbons. After isolation of the new compounds by preparative GC with a cyclodextrin stationary phase the structures were established as guaia-1(10),11-diene (**1**) and guaia-9,11-diene (**2**) by investigation of their 1D and 2D NMR spectra. While relative configurations were established from NOESY experiments, absolute configurations were deduced on the basis of chemical correlations with (+)-γ-gurjunene (**3**) and enantioselective capillary GC analysis using modified cyclodextrin stationary phases.



1



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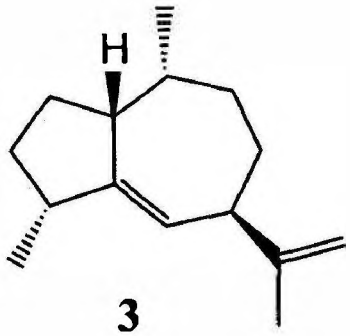

3

P-89

Composition of New *Humulus lupulus* Varietal Essential Oils

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Humulus lupulus (hop) essential oils are primarily used as post-fermentation aroma products in the brewing industry. The aroma quality of a hop variety is often indicated by the caryophyllene to humulene ratio, whereas the bittering potential of a particular hop variety is indicated by the alpha acid content.

The principal hop variety grown in the UK today for downstream brewing products is "Wye Target". "Wye Target" is a conventional height, high alpha, good aroma profile, wilt tolerant hop, which matures late in the hop season. Establishment costs of conventional height hops, however, are very high. Experience has shown that wilt tolerance will be eroded over time. Late maturing varieties are best complemented with early maturing varieties to extend the picking season.

Three new *Humulus lupulus* varieties have recently been grown commercially to address these problems, extending the picking season, improving wilt resistance and decreasing establishment costs by introducing a "dwarf" gene to reduce the internodal distance.

The first of these new varieties "Phoenix" was released in 1996. "Phoenix" is seedling of "Yeoman" and is conventional in height, with a high alpha content, good aroma profile and good wilt tolerance. It also matures early in the season and it is for this reason that it is grown commercially to complement the late season variety "Wye Target".

The second of these new varieties "Pilgrim" was registered in 2001 and has a numbered breeding line parentage. "Pilgrim" is a conventional height variety but is half-sister to the dwarf variety "First Gold", having the same father. This variety is very resistant to wilt, has a high alpha content, good aroma profile and is grown commercially because of its high resistance to wilt. "Pilgrim" rectifies deficiencies in "Wye Target" by good storage of the alpha, having good cone resistance to downy mildew and a 5-15% increase in yield over "Wye Target".

The third of these varieties "Pilot" was also registered in 2001 and is a dwarf height hop bred from open pollination of "Pioneer". It has the same yield as a conventional height variety, is of moderate alpha content, has some wilt resistance and is grown commercially to reduce establishment costs associated with conventional height hops. It does not have a good aroma profile, however, and is only processed as a bittering (alpha) hop.

In contrast to older varieties such as "Wye Target", "Fuggles" and "Goldings", the selinene content of these new varieties is significantly higher and is believed to reflect the narrow genetic base common to these new varieties. The composition of these new varietal hop oils is presented in this paper.

P-90

Rosemary aroma constituents and their enantiomeric ratio in the samples of different origin

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Rosmarinus officinalis L. (Lamiaceae) is a typical Mediteranean species. It is an aromatic herb with an intense pleasant smell. Rosemary oil is widely used by the cosmetic, food and pharmaceutical industires. Many studies have pointed out the variability of the rosemary essential oil composition depending on various factors [1,2]. The characteristic aroma of essential oils is due not only to the composition, but often also to enantiomeric ratio of the components. Rosemary oil consists mostly of chiral compounds. Their enantiomeric ratios were the subject of this investigation. Borneol was one of the main interest so the optical purity of it's minus form can serve in aroma authenticity control [3].

Two samples of cultivated rosemary leaves from experimental growing stations in Poland and four samples supplied from the open market as well as four rosemary aroma preparates were tested. The volatiles were isolate by distillation in Deryng apparatus with addition of known amount of internal standard and separated by GC (Hewlett Packard 6890 instrument) on HP-5 capillary column (30m x 0.35mm x 0.25μm). The chiral resolution was performed with chiral capillary column Restek RtâDex sm (30m x 0.35mm x 0.25μm) taking the same isolates and also with use of solid phase microextraction SPME (PDMS, 50°C, 15min) to speed up the analysis. Olfactometry and sensory profile analysis were done too.

17 components were identified. Among them there were in higher amounts: α-pinene, camphene, β-pinene, eucalyptol (1,8-cineole), camphor, borneol, α-terpineol, t-caryophyllene. Most of these compounds were stated in rosemary by other authors [1-5]. The concentration of the particular compounds as well as concentration of total volatiles varied significantly among the samples dependently on theirs origin. The total volatiles was observed at the range from 7,4 to 40mg/g of leaves, while for eucalyptol from 1.7 to 14,7mg/g. Eucalyptol occured at the highest concentration even over 50% of the total compounds. Borneol was determined at the range from 0.6 to 1.6mg/g, what corresponded to 4-8% of total volatiles.

Olfactometry measurments revealed eucalyptol, camphor and borneol as the most important constituents for rosemary flavour. In sensory profiles the dominating attributes were eucalyptus-like, camphoraceous, green-grassy and earthy. Principal Component Analysis of sensory data showed significant differentiation between the analysed samples of rosemary leaves.

The chiral analysis allowed to separate 11 pairs of enatiomers. Most of them showed variability of enantiomeric ratio dependently on the sample origin without characteristic excess of one optical form. Borneol was the only one component occured with stable and high optical purity of minus form (-)-1S,2R,4S, not lower than 85%. The SPME method used for chiral separation gave the same results for enantiomeric ratios in comparison with distillates. The method is simple and no time consuming. Therefore it can be valuable tool in aroma control system. It was used for testing four rosemary aroma preparates. In spite of some differences in all of them the high optical purity of (-)-1S,2R,4S borneol was stated, what means the natural origin of these aroma products.

1. Falmini G., Cioni P.L., Morelli I., Macchia M., Ceccarini L., J.Agric. Food Chem., 50, 3512-3517, 2002

2. Serano E., Palma J., Tinoco T., Venacio F., Martins A. J Essent. Oil. Res., 14, 87-92, 2002
3. Mosandl A., Food Rev., 11, 1995
4. Bicchi C., Drigo S., Rublio P., J. Chromatog. A, 892, 469-485, 2000
5. Kaloustan J., Portugal H., Pauli A.M., Pastor J., Journal of Applied Polymer Science, 83, 747-756, 2002

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Enantiomeric Behaviour of 2-Methyl Butyric Acid During its Yeast´s Bioconversion from 2-Methyl Butanol and During its Esterification by Enzymatic or Physical Treatment

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Natural 2-methyl butyric acid (MBA) coming from plants or microrganisms can exist under two enantiomeric forms: predominantly (S)-(+) and also (R)-(-).
One yeast of our Collection, *Saccharomyces cerevisiae*, 92154, gives 99% (S)-(+) enantiomer when the used substrate, 2-methyl butanol, is 99% (S)-(-).
The kinetic of the bioconversion of the strain 92154 has been studied and chiral analysis of MBA have been made during all the process.
Compared to our strain, bioconversions made with bacteria (*Gluconobacter roseus* or *Gluconobacter oxydans*) gives rise to 90-95% (S)-(+) and 5-10% (R)-(-) enantiomers, even if the used substrate is 99% (S)-(-). Our yeast strain, 92154, produces a MBA whose chiral profile correspond to those found in plant. After esterification with ethyl alcohol, MBA 99 % (S)-(+) gives ethyl-2-methyl butyrate (EMB), also 99% (S)-(+), if microbial lipase is used (Lipase of *Candida antarctica*).
The same result is obtained when physical treatment (150°C, 10 bars), without catalyst, is applied to the acid-alcohol system. Other treatments at higher temperature and higher pressure result in racemisation of the MBA and EMB. Kinetics of all these conversions have been followed by chiral analysis.
Natural MBA and natural EMB synthesized by yeast bioconversion and enzymatic reaction (or soft physical treatment) have the same chirality as reported for plant extracts.

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[i] Phokas, G.; Patouha-Volioti, G.; Katsiotis, S., *Studies on the essential oil of the leaves of Micromeria juliana (Labiatae)*, Sect. Pharm., Fr. Plantes Medicinales et Phytotherapie (1980), **14** (3), 159-63.

[ii] Ninkov Dusan, *Composition containing organic phenols for treatment of infections of humans and animals*, Patent, (2001), Application: WO 2000-US22640 20000817

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34th INTERNATIONAL SYMPOSIUM ON ESSENTIAL OILS

ISEO 2003

September 7-10, 2003
Würzburg, Germany

Second Circular

Organization:

Prof. Dr. K.-H. Kubeczka
Prof. Dr. P. Schreier
University of Würzburg

(http://www.pzlc.uni-wuerzburg.de/iseo2003.htm)

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34th INTERNATIONAL SYMPOSIUM ON ESSENTIAL OILS

Organizing Committee

K.-H. Kubeczka P. Schreier, Würzburg

General Information

With the second circular we are pleased to give you more information on the 34th International Symposium on Essential Oils (ISEO 2003) in Würzburg to facilitate your decision to attend the symposium. You are cordially invited to fill in the enclosed registration and accomodation forms as soon as possible. Only those participants who have registered and paid their fees will be allowed to attend the congress. The official language of the symposium is English.

Scientific Program – The following plenary lectures are scheduled:

1. R. NÄF (Geneva/Switzerland)
   The complex chemistry of Camellia sinensis
2. W.A. KÖNIG (Hamburg/Germany)
   Strategies for the identification of known and unknown essential oil constituents
3. P. SCHREIER (Würzburg/Germany)
   Progress in multi-element gas chromatography-isotope ratio mass spectrometry (HRGC-IRMS)
4. R. ANTON (Strasbourg/France)
   Pharmacotoxicology and safety aspects of essential oils
5. W. Schwab (Munich/Germany)
   Molecular biology: An indispensable tool for flavor research

In addition, several oral communications (20 min.) and posters have been announced. In any case, the final decision of the scientific committee and instructions will be made directly to those who have announced a presentation. The abstracts have to be submitted by e-mail.

Final deadline for submission of abstracts is **June 30, 2003**

PROVISIONAL PROGRAM

Sunday, September 7, 2003

17.00 - 19.00	Registration at the Congress Office
19.00 - 21.00	Get-Together-Party (Residenz-Gaststätten, Würzburg, Residenz-platz 1)

Monday, September 8, 2003

9.00 - 9.30	Registration at the Congress Office
9.30 - 10.00	Opening Session
10.15 - 12.00	Scientific communications
14.00 - 18.00	Scientific communications and informal poster session

Tueday, September 9, 2003

9.00 - 12.00	Scientific communications and informal poster session
14.00 - 17.00	Scientific communications and informal poster session
19.00	Symposium Dinner

Wednesday, September 10, 2003

9.00 - 12.30	Scientific communications
14.00 - 19.00	Half-day excursion „Weikersheim Castle“

General Information

Location and time

The get-together-party is in the center of the city, Residenz-Gaststätten, Residenzplatz 1.
The conference and the poster session will be held in the Chemistry central building of the University of Würzburg (Am Hubland). A map of the university area is overleaf.

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Congress office

Sunday, September 7th, 2003, 17.00 – 19.00 in the „Residenz-Gaststätten, Würzburg, Residenzplatz 1.
From Monday 9.00 to Wednesday 12.00 in the Chemistry central building of the University of Würzburg, Am Hubland.

Registration

Registration forms are enclosed.
The registration fee is € 230,- by June 30, 2003 for participants, € 100,- for accompanying persons, and € 60,- for students with legitimation. All charges due to bank transfer have to be paid by the participants. The fee includes one copy of lecture and poster abstracts and attendance at the get-together party.
In addition, for participants and accompanying persons attendance of the congress dinner.

Accomodation

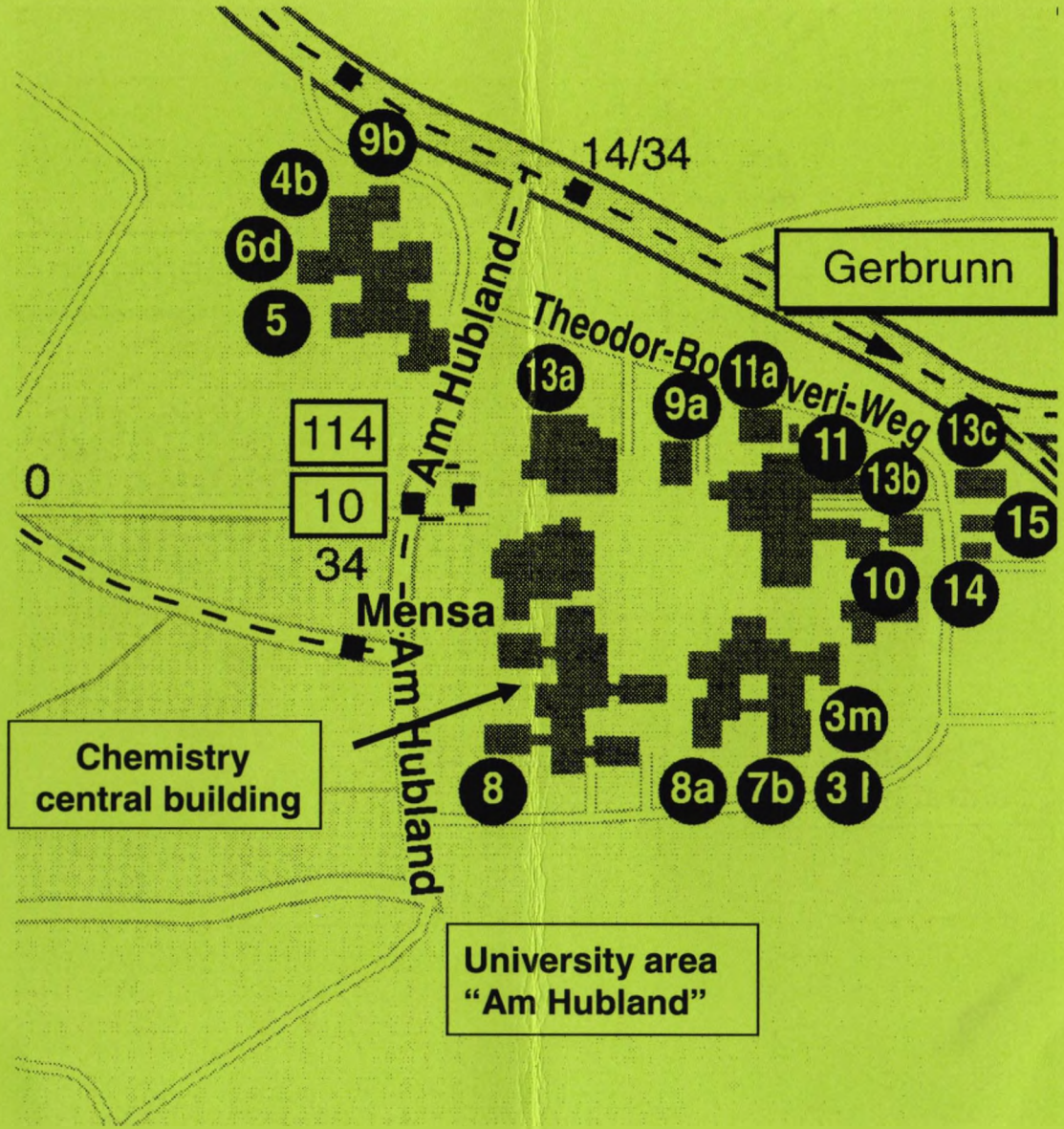
Registrants are expected to make their own arrangements for hotel accomodations. Reservation forms are enclosed. All participants are requested to follow strictly the rules for any change or cancellation indicated in the confirmation letter you will get from the „Congress-Tourismus-Wirtschaft, Würzburg". **The organizers are in no respect responsible for any accomodation poblem.**

Abstracts

Participants wishing to present a communication or a poster are requested to submit an abstract in English of about 200 words (preferably by e-mail to: kubeczka@t-online.de) **not later than June 30, 2003.** Underline the speaker if more than one author.

Poster presentation

The poster boards will be approximately 1.20 (wide) to 1.00 m (hight).



8 Faculty of Chemistry and Pharmacy

Bus-stops:

10 Sanderring
14 Main station (Hauptbahnhof)
34 Heidingsfeld
114 Barbarossa-Platz