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SCIENTIFIC AND SOCIAL PROGRAM

SATURDAY, DECEMBER 7

09:00 Short courses registration and FCT NOVA

1. *Sample preparation methods for chromatographic analysis*. **9:30 to 12:30**
   Eduardo Mateus, Resolution Lab, CENSE-FCT-NOVA, Portugal

2. *MS hyphenation with LC and GC*. **14:30 to 17:30**
   Marco Gomes da Silva, Resolution Lab, LAQV-FCT NOVA, Portugal

3. *Validation of Chromatographic Methods*. **14:30 to 17:30**
   Alice Mosca – AIM, Portugal and Ricardo Bettencourt Silva – FCUL, Portugal

SUNDAY, DECEMBER 8

4. *Comprehensive gas chromatography – GC x GC*. **9:30 to 12:30**
   Philip Marriott, School of Chemistry, Faculty of Science at Monash University – Australia
5. *HPLC*. **14:30 to 17:30**
   Marco Gomes da Silva, Resolution Lab, LAQV-FCT NOVA, - Portugal

WEDNESDAY, DECEMBER 11

6. *Large-scale efficient extraction of chemical information from untargeted chemical profiling (GC/MS) data*. **14:30 to 17:30**
   Rasmus Bro, Copenhagen University, Faculty of Sciences – Denmark

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P23***Monitoring tranexamic acid in human urine by automatic solid-phase extraction combined with liquid chromatography-mass spectrometry*** *Fernandes SR, Barreiros L, Sá P, Miró M, Segundo MA*	**79**
P24 ***Analysis of Environmental Contaminants in Smoked and Cured Codfish Samples*** *Ramalhosa MJ, Paíga P, Teixeira S, Delerue-Matos C*	**80**
P25 ***Assessment of Contaminants in Salmon Using QuEChERS Methodology and Liquid Chromatography*** Paíga P, Ramalhosa MJ, Teixeira S, Delerue-Matos C	**81**
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P33 Comparison of the volatile profile of the essential oils extracted from the aerial parts and roots of lovage (*Levisticum officinale* W.D.J. Koch)

Rafael Mascoloti Sprea,[1,2] Cristiane Canan,[2] Lillian Barros,[1] Isabel C. F. R. Ferreira,[1] Joana S. Amaral [1,3,*]

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Lovage (*Levisticum officinale* W.D.J. Koch.) is a perennial aromatic plant from the Apiaceae (Umbelliferae) family cultivated in several European countries. The aerial parts of this plant are used in culinary due to their strong taste like celery combined with parsley with a scent of aniseed and curry. The aroma and flavour of the aerial parts of the plant somehow remember some commercial condiments, therefore being commonly designated in Portugal as "planta do knorr" and in several countries as "Maggi plant". [1] Although, currently, other aromatic herbs from the same family are much more used than lovage, this species was once much recognized, being considerably used either by the condiment's industry [2] as well as by households in soups, stews, meat dishes, etc. The root of *L. officinale* has been known for centuries as a traditional medicine possessing carminative and spasmolytic activity [3] and is also known to contain essential oils in its composition. It has been described to present also a warm-spicy note, although not as intense as the leaves and seeds.
In this work, the volatile profile of the essential oils extracted from edible aerial parts and roots of lovage were determined. Fresh aerial parts (leaves and stems) were commercially acquired in 2018 at Porto, Portugal, while the roots were obtained dried, being acquired from an herbal shop in Spain. The essential oil was extracted by hydrodistillation in a Clevenger apparatus in accordance with the European Pharmacopoeia. Because of the low yield obtained for the root's oil, 2 mL of hexane were added to the distilled mixture of water/essential oil. The oil from the aerial parts was recovered directly without adding any solvent. Samples were analysed in a GC-2010 Plus (Shimadzu) gas chromatography system with a AOC-20iPlus automatic injector and a mass spectrometry detector. Separation was achieved on a SH- RXi-5ms column (30 m x 0.25 mm x 0.25 µm; Shimadzu, USA). Compounds identification was based on the NIST17 mass spectral library and in the linear retention index calculated based on the retention times obtained for a reference mixture of *n*-alkanes. Comparisons were also performed with published data and, when possible, with commercial standards. Quantification was performed as relative percentage of total volatiles using relative peak area values obtained directly from the total ion current (TIC) values.
GC–MS analysis enabled the identification 99.1% of compounds, corresponding to a total of 44 identified compounds in the aerial parts, those belonging mainly to monoterpenes (74.0%) and phthalides (24.3%). α-Terpinyl acetate was found to be the major compound (33.6%), followed by *p*-cymene (20.5%), (*Z*)-ligustilide (22.2%), β-phellandrene (4.7%) and myrcene (4.2%). For the root's a total of 60 compounds were identified, corresponding to a total of 88.4%, with the phthalides group being the major group (61.7%). Different phthalides were present, being (*Z*)-butylidenephthalide (29.0%) the major compound, followed by neocnidilide (8.9%) and (*Z*)-ligustilide (8.5%). Among the remaining compounds, the sesquiterpene alcohol spathulenol (6.3%) was the one in higher amounts. The obtained results evidence the presence of high amounts of phthalides in the essential oils of both botanical parts of lovage. Phthalides are believed to play a major role in the aroma of lovage. [3] Moreover, different biological properties, including antioxidant activity, antihyperglycemic activity, analgesic and neurological effects, have been ascribed to these compounds, in particular to (Z)-ligustilide, which can support the use of lovage, particularly the roots, use in traditional medicine.

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