

# BOOK OF ABSTRACTS



30 Aug – 3 Sept, Figueira da Foz, Portugal

http://csi2015.fis.uc.pt

#### Welcome

Colloquium Spectroscopicum Internationale XXXIX is a conference series which is held every two years in a different country. The first one happened in Strasbourg, France, 1950, and the former one in Tromsø, Norway, 2013.

This symposium endeavors to congregate physicists and chemists from universities and research institutions with industry analysts in all fields of analytical spectroscopy, centering the discussion not only on the results of basic research and method development but also on the outcome from daily practice in the field of optical spectroscopy. The Local Organizing Committee of the Colloquium Spectroscopicum Internationale XXXIX (CSI 2015) is pleased to welcome all participants in Figueira da Foz, Portugal.

CSI2015 will be held in "CAE - Centro de Artes e Espectáculos", Figueira da Foz, a modern Conference Hall with pleasant ample space, including an inner garden with glazed roof.

About 280 delegates from 36 countries will have the opportunity to exchange ideas and knowledge related to all fields of analytical spectroscopy, centering the discussion not only on the results of basic research and method development but also on the outcome from daily practice in the field of optical spectroscopy.

The conference programme will consist of 14 plenary lectures and 11 keynote lectures from distinguished scientists, 82 oral presentations and 204 poster contributions.

We thank our sponsors and all the people that contributed for this event to take place. We hope that you enjoy your participation in CSI 2015.

On behalf of the Local Organizing Committee, Maria Luísa de Carvalho Joaquim M. F. dos Santos

Cristina M. B. Monteiro

Conference Web-page: <u>http://csi2015.fis.uc.pt/</u>

E-mail: <u>csi2015@fis.uc.pt</u>

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## **Scientific Topics**

- A Atomic spectrometry (ICP OES, ICP-MS, GD, AAS, etc.);
- B Molecular spectrometry (UV-Vis, NMR, Raman, IR, etc.);
- C Organic and inorganic mass spectrometry (TIMS, MALDI, LC-MS, GC-MS);
- D X-ray spectrometry (XRF, XRD, XANES, PIXE, etc.);
- E Hyphenated techniques;
- F Laser spectroscopy;
- G Imaging techniques;
- H Nuclear techniques (Mössbauer spectroscopy, Gamma spectroscopy, NAA);
  I Methods of surface analysis and depth profiling;
- J Application of spectroscopy in:
- J1 Material sciences (nano/micro, surface and interface analysis);
- J2 Environmental and geochemical analysis;
- J3 Archaeometry and cultural heritage;
- J4 Biological applications;
- J5 Food analysis;
- J6 Clinical and pharmaceutical analysis;
- J7 Speciation analysis/Metallomics;
- J8 Mass spectrometry in post-genomics and proteomics;
- J9 Miniaturisation and nanotechnology;
- J10 Fuels and biofuels; Recent Scientific Developments by XRS Instrumentation

#### **Invited Speakers**

Randolf Pohl	Opening Talk, Monday 09:15
Max-Planck-Institute of Quantum Optics, Germany	
Alfredo Sanz Medel	CSI Award, Tuesday 08:45
University of Oviedo, Spain	
JJ Gomez Cadenas	Topic H, Monday 10:35
IFIC, CSIC & Universitat de València, Spain	
Patrick J. Parsons	Topic C, Monday 14:30
Wadsworth Center and University at Albany, USA	
Gary Hieftje	Topic B, Tuesday 09:30
Indiana University, USA	
György Tarczay	Topic B, Tuesday 10:35
Eötvös University, Hungary	
Luo Liqiang	Topic D, Tuesday 14:30
National Research Center of Geoanalysis, China	
Koen Janssens	Topic J3, Wednesday 08:45
AXES Research Group, University of Antwerp, Belgium	
Jose M. Costa-Fernandez	Topic J9, Wednesday 09:30
University of Oviedo, Spain	
Patricia Smichowski	Topic J2, Wednesday 10:35
Comisión Nacional de Energia Atômica, Argentina	
CEDALA and University of Careerings Dravil	Topic J7, Thursday 08:45
GEPAM and University of Campinas, Brazil	Tamia F. Thursday, 00:20
CNR Institute of Chemistry of Organometallic Compounds, Italy	Topic E, Inursday 09:30
Parbara Waapar	Topic 12 Thursday 10:25
University of Warsaw Poland	Topic 33, morsady 10.35
	Topic P. Thursday 14:00
Taras Shevchenko National University of Kviv, Ukraine	
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## **Keynote Speakers**

Margaretha De Loos Vollebregt Ghent University, Belgium	Topic A, Monday 11:25
René Van Grieken University of Antwerp, Belgium	Topic J3, Monday 11:25
<b>Yngvar Thomassen</b> National Institute of Occupational Health, Norway	Topic J2, Monday 11:25
<b>Jun Kawai</b> Kyoto University, Japan	Topic D, Monday 11:25
Alessandro D'Ulivo Institute of Chemistry of Organometallic Compound, Italy	Topic A, Tuesday 11:25
<b>Robert McCrindle</b> Tshwane University of Technology, South Africa	Topic J2, Tuesday 11:25
<b>Ryszard Łobiński</b> National Research Council of France, France	Topic B, Tuesday 11:25
<b>Ewa Bulska</b> University of Warsaw, Poland	Topic J4, Tuesday 11:25
Jiri Dědina Institute of Analytical Chemistry of the ASCR, Czech Republic	Topic A, Thursday 11:15
<b>Bernhard Welz</b> Universidade Federal de Santa Catarina, Brazil	Topic C, Thursday 11:15
Alexander A. Kamnev Russian Academy of Sciences, Russia	Topic H, Thursday 11:15

## Proceedings of the CSI 2015

The Proceedings will be published, following peer review, in the **Spectrochimica Acta B** and in the **Spectrochimica Acta A** Journals.

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## Determination of carboxylic acids in biological matrices by GC/MS following single-step aqueous derivatization with triethyloxonium tetrafluoroborate

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The accurate determination of carboxylic acids in biological matrices is crucial for understanding metabolic pathways related to plant growth and development [1] and for the determination of i) biomarkers of bacterial activity in food and environmental samples (e.g. salicylic, propionic, and butyric acid) [2], ii) drug metabolites such as salicylic acid for aspirin [3], and iii) environmental pollutants associated with adverse health effects like the perfluorooctanoic acid [4-5].

In this study, the determination of several organic acids was achieved by GC/MS following a single-step aqueous derivatization with triethyloxonium tetrafluoroborate. Conversion of the carboxylic acids into the corresponding ethyl-esters was attained for indole-3-acetic acid, benzoic acid, salicylic acid, propionic acid, butyric acid and perfluorooctanoic acid.

Before derivatization and quantitation, these analytes were simultaneously extracted in a slightly alkaline solution from various matrices such as *Nicotiana tabacum* and *Actinidia deliciosa* leaves, urine, and saliva. Compared to common derivatization approaches for GC analysis, the proposed method has the advantage to be based on a simple aqueous chemistry. In this regard, the sample preparation involves only centrifugation, aqueous derivatization and liquid-liquid extraction of the resulting ethyl-esters with MTBE. Optimization of some effective parameters for the derivatization step – such as pH of the reaction medium, amount of reagent, and derivatization/extraction time – was established. For the utmost precision, quantitation was performed based on isotope dilution formalism by using deuterated internal standards. Linearity, repeatability, recovery, limit of detection and quantitation were evaluated for each analyte under investigation, along with the matrix effects.

#### References

[1] Y. Bai, D. Fuyou, and L. Huwei, Analytical Methods, 2, 1867-1873 (2010).

[2] N.M. Moreau, R. Delépée, D. Maume, B. Le Bizec, P.G. Nguyen, M.M. Champ, L.J. Martin, and H.J. Dumon, Analytica chimica acta, 512, 305-310 (2004).

[3] M. T. Jafari, Z. Badihi, and E. Jazan, Talanta, 99, 520-526 (2012).

[4] S.D. Richardson, T.A. Ternes, Analytical Chemistry, 86, 2813-2848 (2014).

[5] J. Koponen, P. Rantakokko, R. Airaksinen, and H. Kiviranta, Journal of Chromatography A, 1309, 48-55 (2013).