



August 29
Auditorium

Monday

Aug 29

14:30 H **Registration Opens**

16:00 H **Opening Ceremony**

16:30 H **Medical Diagnosis**

Chairman: J. J. C. Teixeira-Dias *Aveiro University (Portugal)*

Plenary Lecture: Max Diem *Northeastern University (USA)*
Spectral Histopathology (SHP) and Spectral Cytopathology (SCP):
Applications of Infrared Microspectroscopy in Medical Diagnostics

Invited Lecture: Ganesh Sockalingum *University of Reims Champagne-Ardenne (France)*
Vibrational Spectroscopy and Imaging, a Promising Tool Towards Spectral
Cytology: Monitoring Drug-cell Interaction at the Single Cell Level

Oral: Anthony Parker *STFC Rutherford Appleton Laboratory (UK)*
Spatially Offset Raman Spectroscopy Towards Diagnosing Bone Disease
- an Update

19:00 H ***St. Michael Chapel Concert***
University of Coimbra

19:45 H ***Welcome Cocktail***
Weapons Room, Rectorate of the University of Coimbra

August 30
Auditorium



09:00 H **Synchrotron Radiation Spectroscopies**

Chairman: **Timothy Keiderling** *University of Illinois at Chicago (USA)*

Plenary Lecture: **Peter Gardner** *University of Manchester (UK)*
Infrared Spectroscopic Analysis of Single Biological Cells: The Case for
Scattering Correction

Invited Lecture: **Eugen Stulz** *University of Southampton (UK)*
Circular Dichroism

10:30 H *Coffee break*

11:00 H **Vibrational Spectroscopies**

Chairman: **Steven Boxer** *Stanford University (USA)*

Invited Lecture: **Santiago Sanchez-Cortes** *IEM-CSIC (Spain)*
Plasmonics Helps Spectroscopy to Understand Biomolecules

Invited Lecture: **Janina Kneipp** *Humboldt-University at Berlin (Germany)*
Surface-enhanced RAMAN Scattering of Cells and Other Biomaterials

Short Oral: **Eric Guittet** *CNRS (France)*
Integrated Structural Biology Shows How Scare Sequence Elements Control
the Function of Single β -Thymosin/WH2 Domains in Actin Assembly

Short Oral: **Tanja Dučić** *DESY Hamburg (Germany)*
Manganese Compartmentalisation and Oxidative Status on the Cellular
Level of Two Different Plants Lines

Short Oral: **Ariel Guerrero** *University of Windsor (Canada)*
Surface-enhanced RAMAN Scattering of the CLPFFD-NH₂ Peptide
and Two Isomers

Short Oral: **Salim Abdali** *University of Copenhagen (Denmark)*
SERS and SEROA for Biological Molecules Detection and Diagnostic

13:00 H *Lunch*

Aug 30

Tuesday



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14:30 H Vibrational Spectroscopies

Chairman: Armida Torreggiani *ISOF, National Research Council - CNR (Italy)*

Plenary Lecture: Mischa Bonn *FOM-Institute AMOLF (The Netherlands)*

Label-free, Real-time Studies on Intermolecular Interactions at Model Membranes using Surface Vibrational Spectroscopy

Invited Lecture: Klaus Gerwert *Ruhr-University Bochum (Germany)*

Vibrational Micro(spectro)scopy at Different Scales: Proteins, Membranes and Living Cells

Short Oral: Karin Hauser *University of Konstanz (Germany)*

Mechanisms of Protein Folding Studied by Time-resolved Temperature-jump IR-Spectroscopy

Short Oral: Emilie Bulard *University of Paris Sud 11 - ISMO (France)*

The Effect of Bacterial Adhesion on Grafted Chains Revealed by the Non Invasive Sum Frequency Generation (SFG) Spectroscopy

16:30 H Coffee break

17:00 H Vibrational Spectroscopies

Chairman: Andreas Barth *Stockholm University (Sweden)*

Invited Lecture: Achim Kohler *Norwegian University for Life Sciences (Norway)*

Calibrating FTIR Spectra for Fatty Acid Profiles of Cells
– Opportunities and Challenges

Short Oral: Allison Derenne *University Libre of Bruxelles (Belgium)*

Effect of Anticancer Drugs of Different Cell Lines Classified by FTIR Spectroscopy

Short Oral: Marie-Laure Brandily *University of Rennes (France)*

Optical Fiber Probe for Infrared Food Safety and Medical Diagnosis

18:00 H Poster Session I

19:00 H Odd numbers

August 31
Auditorium



09:00 H

Neutron Techniques

Chairman: **Hugh D. Burrows** *Coimbra University (Portugal)*

Plenary Lecture: John Tomkinson *The ISIS Facility, STFC (UK)*
The Role of Neutron Spectroscopy in the Study of Biomolecules

Invited Lecture: Gregory Chass *University of Wales, Bangor (UK)*
Systems Chemistry: Cooperative Low-Energy Dynamics Driving Reactivity and Selectivity, Probed by Neutrons and Muons

Short Oral: Daniela Russo *CNR (France)*
Vibrational Density of States on Hydration Water at Biomolecular Sites: Hydrophobicity Promotes Low Density Amorphous Ice Behaviour

Short Oral: Wiebke Knoll *Institut Laue-Langevin (France)*
Exploring the Brain with Neutrons

11:00 H

Coffee break

11:30 H

Theoretical Approach

Chairman: **Manuel Dauchez** *University of Reims Champagne-Ardenne (France)*

Oral: Solomon Stavrov *Tel Aviv University (Israel)*
Mössbauer Spectroscopy as a Probe of the Electric Field in Deoxyheme Proteins: Theoretical Approach

Short Oral: Valery Andrushchenko *Academy of Sciences (Czech Republic)*
Supramolecular Structure of Diolein and Stearyl Alcohol Characterised by IR Spectroscopy and Theoretical

Short Oral: Francisco Partal Ureña *University of Jaén (Spain)*
Molecular Structure and Spectral Features of Mixed-Ligand Metal Ion Complexes that Contain Cu^{2+} , Alanine, Cl^- and Water

12:30 H

Lunch

13:30 H

Organised Sightseeing
Visiting Luso and Buçaco

Aug 31

Wednesday



September 01
Auditorium

09:00 H **Ultra-Fast Techniques**

Chairman: **John Tomkinson** *The ISIS Facility, STFC (UK)*

Plenary Lecture: C. Chatgililoglu *ISOF (Italy)*

Chemical Radiation Studies Related to Radical-based DNA Damage

Invited Lecture: Jasper van Thor *Imperial College London (UK)*

Ultrafast Vibrational Dynamics of Parallel Excited State Proton Transfer Reactions in the Green Fluorescent Protein

10:30 H *Coffee break*

11:00 H **Imaging live cells**

Chairman: **Max Diem** *Northeastern University (USA)*

Oral: Roger Bisby *University of Salford (UK)*

Multiphoton-excited Fluorescence Lifetime Imaging for Study of Intracellular Uptake of Biomolecules and Drugs

Oral: Ioan Notinger *University of Nottingham (UK)*

Label-free Imaging of Phenotypic Spectral Markers in Live Cells Derived from Human Stem Cells

Short Oral: Liesbeth Hartsuiker *University of Twente (The Netherlands)*

Visualising Gold Nanorods and their Broadband Emission in Breast Cancer Cells

Short Oral: Sebastian Dochow *Institut of Photonic Technologie (Germany)*

RAMAN Activated Cell Sorting in Micro Fluidic Chips for Identification of Circulating Tumor Cells

Short Oral: Michael Mengqiu Li *University of Sheffield (UK)*

Rapid Resonance RAMAN Micro-spectroscopy to Probe Carbon Dioxide Fixation in Microbial Single Cells

12:30 H *Lunch*

Thursday

Sep 01

September 01
Auditorium



14:00 H **Luminescence Techniques**

Chairman: **Jasper van Thor** *Imperial College London (UK)*

Plenary Lecture: **Hugh D. Burrows** *Coimbra University (Portugal)*

Using Luminescent Conjugated Polymers to Probe Biologically Relevant Molecules

Invited Lecture: **Jerker Widengren** *KTH Royal Institute of Technology (Sweden)*

Transient State Monitoring - Approaches and Possible Benefits for Biomolecular Studies

Short Oral: **Pascale Chaugenet-Barret** *CNRS (France)*

Intrinsic Fluorescence Properties of DNA G-Quadruplex Structures

Short Oral: **Inês Torcato** *Lisbon University of Medicine (Portugal)*

Novel Antimicrobial Peptides with Activity Against Gram-negative and Gram-positive Bacteria

16:00 H **Coffee break**

16:30 H **Chiroptical Spectroscopy**

Chairman: **Peter Gardner** *University of Manchester (UK)*

Invited Lecture: **Mahmoud Ghomi** *University of Paris 13 (France)*

Structure-activity Relationships of Peptides with Therapeutic Interest

Oral: **Giuliano Siligardi** *Diamond Light Source (UK)*

Diamond B23 Synchrotron Radiation Circular Dichroism Beamline and its Applications in Biostability, Ligand Interactions and in Micro- and Nano-materials

Short Oral: **Günnur Güler** *University of Goethe (Germany)*

Real Time Observation of Proteolysis with Fourier Transform Infrared (FT-IR) and UV-Circular Dichroism Spectroscopy: Watching a Protease Eat a Protein

Short Oral: **Elena Chikhirzhina** *Institute of Cytology (Russia)*

Structural Bases of the Formation of Supercondensed Sperm Chromatin Revealed by CD Spectroscopy of DNA-H1 Complexes

18:00 H **Poster Session II**

19:00 H Even numbers

Sep 01

Thursday



September 02
Auditorium

09:00 H **Magnetic Resonance Techniques**

Chairman: Alexandre Bonvin *Utrecht University (The Netherlands)*

Plenary Lecture: Isabel Moura *New University of Lisbon (Portugal)*
Bioinorganic Aspects of Denitrification

Invited Lecture: Ana Gil *Aveiro University (Portugal)*
Can Biofluids Metabolic Profiling Help to Improve Healthcare during Pregnancy?

Invited Lecture: João Pedro Duarte *Coimbra University (Portugal)*
Probing Organic Semiconductors with Muon Spin Rotation (μ SR), an Exotic Experimental Analogue of NMR

11:00 H *Coffee break*

11:30 H
13:00 H **WorkShop AGILENT**

13:00 H *Lunch*

14:30 H **Magnetic Resonance Techniques**

Chairman: Jan Raap *Leiden Institute of Chemistry (The Netherlands)*

Plenary Lecture: Alexandre Bonvin *Utrecht University (The Netherlands)*
Building Macromolecular Assemblies by Information-driven Docking.
Challenges and Perspectives

Invited Lecture: Margarida Castro *Coimbra University (Portugal)*
The Promising Pharmacological Properties of a Vanadium Compound
as Assessed by *in vivo* Magnetic Resonance Studies

Short Oral: Aureliano Alves *University of Algarve (Portugal)*
Spectroscopic Studies of Vanadate, Decavanate and Vanadyl Interaction
with Actin

Short Oral: K. Kristoffer Andersson *University of Oslo (Norway)*
Spectroscopic and DFT Studies of the Tyrosyl Radicals and the Binuclear
Metal-ion Sites in R2F/R2 Subunits of Ribonucleotide Reductase

Short Oral: Ana Maria Silva *C. Neurosciences and Cell Biology (Portugal)*
 ^2H NMR Analyses of Hepatic Glutamate and Triglycerides: a Window
to Liver *De Novo* Lipogenesis Assessment

17:00 H **Meeting of the Scientific Committee**

20:30 H *Conference Dinner at Convent of Sandelgas*

Friday
Sep 02

September 03
Auditorium



09:00 H	<p>Chairman: Mahmoud Ghomi <i>University of Paris 13 (France)</i></p> <p>Plenary Lecture: Steven Boxer <i>Stanford University (USA)</i> Electrostatics and Dynamics in Proteins using Vibrational Stark Spectroscopy</p> <p>Short Oral: Gal Schkolnik <i>Technical University Berlin (Germany)</i> Probing Electric Fields in Cytochrome c using the Vibrational Stark Effect</p> <p>Short Oral: Miguel Pleitez <i>Goethe University (Germany)</i> Photoacoustic Spectroscopy of Glucose using a Pulsed Tunable Quantum Cascade Laser: Advances Towards the Non-invasive Glucose Measurement in Intracutaneous Liquid</p>
10:30 H	<i>Coffee break</i>
11:00 H	<p>Chairman: Anthony Parker <i>STFC Rutherford Appleton Laboratory (UK)</i></p> <p>Oral: Jan Raap <i>Leiden Institute of Chemistry (The Netherlands)</i> Pulsed ESR Study of the Topology and Dynamics of a Spin-labelled Lipopeptide Antibiotic in Lipid Membrane</p> <p>Invited Lecture: Timothy Keiderling <i>University of Illinois at Chicago (USA)</i> β-Sheets: Hairpins and Design Oligomers to Aggregates and Fibrils, Spectroscopic Stability and Structure Studies</p>
12:00 H	<i>Closing Ceremony and Student Prizes Awarding</i>

Sep 03

Saturday