# Tuesday 30<sup>th</sup> August 2022

8h45-10h15		ISOTOPIC LABELLING
		Chair: Maria Paula MARQUES
	8h45	Invited speaker: Howbeer MUHAMADALI
		Spectroscopic probing of bacterial metabolism at single-cell level
	9h15	Christophe SANDT
		Do Galleria mellonella larvae metabolize polyethylene? An FTIR
	01.20	microspectroscopy study using isotopoic labelling
	9h30	Giulia GIUBERTONI
		Strong isotope-effect on the conformation and self-assembly of collagen
	9h45	
	JIIIJ	Labelling endothelial cells with Raman probes improves the
		specificity and sensitivity of their imaging
	10h00	Stephan PISSOT*
		Rapid antibiotic susceptibility testing using FTIR spectroscopy and
		deuterium isotope probing
10h15	-10h45	INDUSTRIAL SPONSORS
		Chair : Ali TFAYLI
	10h15	ENDRESSHAUSER -KAISER
	10h25	METROHM
	10h35	OPTON LASER INTERNATIONAL
10645	-11h15	Coffee break
		ENHANCEMENT TECHNIQUES
	-12h45	
	-12h45	Chair: Igor CHOURPA
		Chair: Igor CHOURPA Invited speaker: Alois BONIFACIO
	-12h45	Chair: Igor CHOURPA Invited speaker: Alois BONIFACIO Label-free SERS spectra of biological samples: characteristics and
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	14h45	Ewelina BIK*		
		Drug induced phospholipidosis in endothelial cells studied by		
		Raman imaging		
	15h00	Nicolas GOFFIN*		
		Characterization of cancer-associated adipocytes by Raman spectroscopy		
	15h15	Karolina ŠIŠKOVÁ		
	101110	Bimetallic Au-Fe(III) nanocomposites for multimodal imaging		
15h30-	-16h00	INDUSTRIAL SPONSORS		
		Chair : Ali TFAYLI		
	15h30	OPTOPRIM		
	15h40	PERKINELMER		
	15h50	PHOTOTHERMAL SCIENTEC		
16h00-	-16h30	Coffee break		
16h30	-17h30	MOLECULAR SPECTROSCOPY 2		
		Chair: Susan QUINN		
	16h30	Invited speaker: Sébastien BONHOMMEAU		
		Tip-enhanced Raman spectroscopy for nanoscale chemical and		
	17h00	structural characterization of biomolecules		
	171100	<b>Monica MARINI</b> Background-free DNA-protein interactions: structural insights by		
		Raman spectroscopy		
	17h15	Stepan JILEK*		
		Raman optical activity as a potent tool for studies of		
		mononucleotide G-quadruplexes		
1/h30	-18h15	FLASH PRESENTATIONS		
		Chair: Francesca PALOMBO and Agnieszka BANAS		
		LASSAAD*		
Monitoring of the accumulation of Squalene-Gemcitabine nanomedic within single living breast cancer cell by Raman imaging				
		ALSHAREEF*		
	Single (	Cell FTIR Imaging with Novel ZnS Hemispheres for Studying		
		lipidosis in Live Macrophages		
		a AUGUSTYNIAK*		
	Early detection of stem cells transformation using FTIR and High-Resolution Raman Imaging			
	SIMIECORR: Mie scatter correction without a prior assumption about the			
	chemical composition of a sample			
	Arianna BONIZZI*			
	Identification of a biochemical signature of dysfunctionality by Raman			
	spectroscopy analysis of lipoproteins Annalisa CARRETTA*			
	From synthetic identity to biological function of a doxorubicin liposoma			
	formulat			
	-			

### Gary COONEY\*

Tip-Enhanced Raman Spectroscopy of Tau fibrils: Measurement and Chemometric Analysis

### Markéta FOUSKOVÁ

Raman Spectroscopy in the Early Diagnosis of Colorectal Cancer

#### Francesca GASPARIN\*

Live-cell Mid-infrared Optoacoustic Microscopy and Spectroscopy for Longitudinal Metabolic Monitoring

### Philip GASSE\*

Two-dimensional infrared spectroscopy of carbohydrates with site-specific reporter groups

### Pooja GIRISH\*

Spectral tissue imaging for ex-vivo cancer diagnosis and survey

### Julien GUILLARD\*

FTIR spectral imaging analysis of cirrhosis development in two murine models

### Mahmoud HULEIHEL

Infrared Spectroscopy in Tandem with Machine Learning for Simultaneous Rapid Identification of Bacteria Isolated Directly from Patients' Urine Samples and Determination of Their Susceptibility to Antibiotics

### Maria KRAJAČIĆ\*

Artificial Neural Network and Support Vector Machine Regression for Forensic Age Determination Using Raman Spectra of Teeth

#### Chen LIU\*

Raman-based Detection of Antibiotics in Pharmaceutical Formulations and Biological Matrices

### Shibarjun MANDAL\*

Bacteria localization in hematogenous osteomyelitis using fluorescence and Raman imaging

### Nathan MEYER\*

Detection of A $\beta$  1-42 aggregates by RT-FAST: toward a new tool for the diagnostic of Alzheimer's disease

### **Pierre NIZET\***

Assessment of Ovarian Tumor Growth in Wild-Type and Lumican-Deficient Mice: Insights Using Infrared Spectral Imaging, Histopathology, and Immunohistochemistry

### Imane OUDAHMANE\*

Vibrational spectroscopy applied on biofluids: infrared spectroscopy for bladder cancer diagnosis using urine samples

### **Ayyoub RAYYAD\***

Analytical quality control of therapeutic mAbs preparations by Raman spectroscopy

### José Javier RUIZ\*

Identification and biochemical characterization of breast cancer cells resistant to neoadjuvant treatment by Raman Spectroscopy

### Oliva SALDANHA

Calcium induced vesicular interactions studied with ATR- FTIR spectroscopy

## František ŠANDA

Lineshape analysis of 2D spectra for fifth order spectroscopies: exciton transport, annihilation and spectral diffusion dynamics

### **Till STENSITZKI**

High-throuput 2D-IR spectroscopy using the HARE chip

### Laurence VAN GULICK

Effects of obesity on the structural organization and mechanical properties of type I collagen

### Clara WATTIEZ\*

Determining the influence of H/D exchange on IR spectroscopy and vibrational dynamics of polypeptide secondary structures

### Martina ZANGARI\*

The role played by protein-asbestos fiber interaction in asbestos pathogenicity

#### 18h15-20h45 **POSTER SESSION – WINE AND CHEESE**

- 1. Samar ADAWI\* Using FTIR-ATR spectroscopic method to monitor the development of fungi in plants and bread 2. Almar AL ASSAAD\* Monitoring of the accumulation of Squalene-Gemcitabine nanomedicine within single living breast cancer cell by Raman imaging 3. **Ohood ALSHAREEF\*** Single Cell FTIR Imaging with Novel ZnS Hemispheres for Studying Phospholipidosis in Live Macrophages 4. Ali ASSAF Monitoring of algal production in photobioreactors by Raman spectroscopy and chemometrics 5. Karolina AUGUSTYNIAK\* Early detection of stem cells transformation using FTIR and High-**Resolution Raman Imaging** Luís BATISTA DE CARVALHO 6. Who's who? Discrimination of Breast Cell Lines by FTIR Microspectroscopy 7. Vladimír BAUMRUK Absolute configuration determination of promising new drug for Parkinson's disease via Raman optical activity Lucie BEDNÁROVÁ 8. Structural Investigation of  $\alpha/\gamma$ -Hybrid Peptide Oligomers 9. Uladzislau BLAZHKO SIMIECORR: Mie scatter correction without a prior assumption about the chemical composition of a sample Arianna BONIZZI\* 10. Identification of a biochemical signature of dysfunctionality by Raman spectroscopy analysis of lipoproteins
- **Radek BURA\*** 11.

Isotopic labeling of microalgae: Raman study

12.	Annalisa CARRETTA* From synthetic identity to biological function of a doxorubicin liposomal formulation
13.	Murali Krishna CHILAKAPATI Raman isotope probing (RIsP) for identifying antimicrobial resistance
14.	Murali Krishna CHILAKAPATI Raman Spectroscopy based metabolomics for bioprocess monitoring
15.	<b>Murali Krishna CHILAKAPATI</b> Raman Spectroscopy Analysis of Plasma of Diabetes Patients without and with Retinopathy, Nephropathy, and Neuropathy
16.	<b>Gary COONEY*</b> Tip-Enhanced Raman Spectroscopy of Tau fibrils: Measurement and Chemometric Analysis
17.	Mohammed ESSENDOUBI Raman Micro-Spectroscopy for skin and hair cosmetics testing
18.	Markéta FOUSKOVÁ Raman Spectroscopy in the Early Diagnosis of Colorectal Cancer
19.	Francesca GASPARIN* Live-cell Mid-infrared Optoacoustic Microscopy and Spectroscopy for Longitudinal Metabolic Monitoring
20.	Philip GASSE* Two-dimensional infrared spectroscopy of carbohydrates with site- specific reporter groups
21.	<b>Pooja GIRISH</b> * Spectral tissue imaging for ex-vivo cancer diagnosis and survey
22.	<b>Giulia GIUBERTONI</b> In situ identification of secondary structures in unpurified Bombyx mori silk fibrils using polarized two-dimensional infrared spectroscopy
23.	<b>Cyril GOBINET</b> Supervised learning of infrared spectral images for the diagnosis of different types of breast cancer
24.	Julien GUILLARD* FTIR spectral imaging analysis of cirrhosis development in two murine models
25.	<b>Petra HELLWIG</b> Vibrational spectroscopies and microscopies: a tool to study and identify neurodegenerative diseases
26.	Mahmoud HULEIHEL Infrared Spectroscopy in Tandem with Machine Learning for Simultaneous Rapid Identification of Bacteria Isolated Directly from Patients' Urine Samples and Determination of Their Susceptibility to Antibiotics
27.	<b>Seydou KANE</b> Reduction of acquisition time in Fourier transform infrared spectroscopy by deep learning

### 28. Hichem KICHOU\*

Analytical performance of Raman spectroscopy for quantification of active ingredients in Human stratum corneum

### 29. Eva KOČIŠOVÁ

Surface-enhanced Raman spectroscopy of biologically important molecules on  $V_2O_5$  nanoparticle films

### 30. Maria KRAJAČIĆ\*

Artificial Neural Network and Support Vector Machine Regression for Forensic Age Determination Using Raman Spectra of Teeth

### 31. Martin KRÁL\*

Infrared s-SNOM imaging of surface adhesive polydopamine layers formed on various substrates

### 32. Kateřina KRÁLOVÁ

Combining Vibrational Spectroscopy, Metabolomics and Proteomics – Comprehensive Analysis of Blood Plasma for Clinical Diagnostics

### 33. Lenka KREPSOVÁ

Photoswitching of Triptycene-Based Molecular Machines Followed by Raman Spectroscopy

### 34. Chen LIU\*

Raman-based Detection of Antibiotics in Pharmaceutical Formulations and Biological Matrices

#### 35. Vanessa LOBOGNON\*

Characterization of Bone-Implant Interface after Osseodensification by Infrared Imaging: Development of an Experimental Model

### 36. Shane MAGUIRE\*

ATR-FTIR spectroscopy of calcium-dependent lipid-binding proteins

### 37. Shibarjun MANDAL\*

Bacteria localization in hematogenous osteomyelitis using fluorescence and Raman imaging

### 38. Lorenz MATTES

Dual-comb-IR-spectroscopy to study temperature-jump dynamics of polyQ model peptides

### 39. Aidan MEADE

Detection of radiosensitive subpopulations ex-vivo via Raman microspectroscopy of lymphocytes

### 40. Nathan MEYER\*

Detection of A $\beta$  1-42 aggregates by RT-FAST: toward a new tool for the diagnostic of Alzheimer's disease

### 41. Pierre NIZET\*

Assessment of Ovarian Tumor Growth in Wild-Type and Lumican-Deficient Mice: Insights Using Infrared Spectral Imaging, Histopathology, and Immunohistochemistry

### 42. Jonas OSHAUG PEDERSEN

Controllable deposition of gold nanoparticles using a one-step centrifugation process and its application for SERS

43.	<b>Imane OUDAHMANE*</b> Vibrational spectroscopy applied on biofluids: infrared spectroscopy for bladder cancer diagnosis using urine samples
44.	<b>Pierre PRADA</b> Identification of circulating biomarkers of Crohn's disease and spondyloarthritis using FTIR spectroscopy
45.	<b>Ayyoub RAYYAD*</b> Analytical quality control of therapeutic mAbs preparations by Raman spectroscopy
46.	<b>Ayyoub RAYYAD*</b> Confocal Raman microspectroscopy as a tool to access the quality of chicken egg
47.	José Javier RUIZ* Identification and biochemical characterization of breast cancer cells resistant to neoadjuvant treatment by Raman Spectroscopy
48.	Oliva SALDANHA* Calcium induced vesicular interactions studied with ATR- FTIR spectroscopy
49.	<b>František ŠANDA</b> Lineshape analysis of 2D spectra for fifth order spectroscopies: exciton transport, annihilation and spectral diffusion dynamics
50.	<b>Christophe SANDT</b> Heterogeneity of human hair medulla lipids, studied by synchrotron µFTIR and OPTIR microspectroscopy
51.	<b>Igor SAZANOVICH</b> ULTRA at Central Laser Facility
52.	<b>Ramona SCHLESINGER</b> The Photoreaction of the Proton-Pumping Rhodopsin 1 from the Maize Pathogen Basidiomycete Ustilago maydis
53.	Karlis SHVIRKSTS Radiation-induced continuous effect on the secondary structure of keratin studied by FTIR spectroscopy
54.	<b>Till STENSITZKI</b> High-throuput 2D-IR spectroscopy using the HARE chip
55.	<b>Paul STRITT*</b> Resolving lipid dynamics in the photocycle of bacteriorhodopsin by mid-IR quantum cascade laser spectroscopy
56.	<b>Daniela TÄUBER</b> Comparative investigation of fibrillar actin using Nano IR spectroscopic and fluorescence microscopy imaging
57.	<b>Laurence VAN GULICK</b> Effects of obesity on the structural organization and mechanical properties of type I collagen
58.	<b>Vincent VAN HEMELRYCK</b> A new convenient tool to analyse protein glycosylation based on FT-IR spectroscopy

### 59. Elise VINCENT

FTIR and biochemical characterisation of glycosaminoglycans (GAGs) content in ovarian cancer cells

### 60. Jehan WAEYTENS\*

Characterization of secondary structure of protein by infrared nanospectroscopy

### 61. Clara WATTIEZ\*

Determining the influence of H/D exchange on IR spectroscopy and vibrational dynamics of polypeptide secondary structures

### 62. Martina ZANGARI\*

The role played by protein-asbestos fiber interaction in asbestos pathogenicity