



Workshop

FTIR Spectroscopy in Microbiological and Medical Diagnostics

Robert Koch-Institute, Berlin
October 10-11, 2019

Venue and Time

Robert Koch-Institute
Nordufer 20, 13353 Berlin, Germany

Registration: October 10, 2019 8:30 – 9:30
Beginning: October 10, 2019 9:30
Ending: October 11, 2019 16:10

Program

Thursday, October 10, 2019

09:30 - 09:40 **Opening remarks**

Session chair: Max Diem

09:40 - 10:00 **Bayden R. Wood** (Clayton, Australia)
Detection of Viral and Immune Response Markers Using Vibrational Spectroscopy

10:05 - 10:25 **Ioan Notingher** (Nottingham, U.K.)
Raman Spectroscopy and Stable Isotope Labelling for Monitoring Host-Pathogen Interaction in Live Cells

- 10:30 - 10:50 **Ute Neugebauer** (Jena, Germany)
Overview of Phenotypic Antibiotic Susceptibility Testing Methods of Pathogenic Bacteria Using Photonic Readout Methods
- 10:55 - 11:25 **Coffee Break**
- Session chair:** Ariane Deniset-Besseau
- 11:25 - 11:40 **Richard A. Dluhy** (Birmingham, USA)
Characterization of Extracellular Vesicles Derived from Red Blood Cells Using Raman Spectroscopy and Machine Learning
- 11:45 - 12:05 **Kang Soo Lee** (Zurich, Switzerland)
Raman Microspectroscopy to Enable Automated Live Sorting of Isotopically Labelled Microbial Cells for Genomics and Ecology
- 12:10 - 12:25 **Natalia Ivleva** (Munich, Germany)
SERS Analysis of Microorganisms: Limitations and Applicability on the Single-Cell Level
- 12:30 - 12:45 **Malama Chisanga** (Manchester, U.K.)
Identification of Industrially Relevant Bacteria in Mixed Microbial Communities Using Raman and SERS Combined with Stable Isotopic Labeling
- 12:50 - 14:00 **Lunch**
- Session chair:** Kamilla Malek
- 14:00 - 14:20 **Maria Paula Marques** (Coimbra, Portugal)
Widening the Frontiers in Forensic Profiling: Probing Burned Human Bones with Neutron and Optical Vibrational Spectroscopy
- 14:25 - 14:45 **Phil Heraud** (Clayton, Australia)
Predicting Growth Temperatures for Southern Ocean Phytoplankton Past and Present Using Infrared Spectroscopy
- 14:50 - 15:05 **Mickael Baqué** (Berlin, Germany)
Supporting Future "Search-for-Life" Missions: Spectroscopy Analysis of Biosignatures After Space and Mars-like Environment Exposure
- 15:10 - 15:25 **Krzysztof Banas** (Singapore, Singapore)
Reliable and Robust Model for Fast Identification and Detection of Counterfeited EBN Products by Using FTIR Microspectroscopy
- 15:30 - 16:00 **Coffee Break**

Session chair: Natalia Ivleva

- 16:00 - 16:15 **Valeria Tafintseva** (Ås, Norway)
Quality Test for FTIR Spectra and Pre-processing of FTIR Images Using
Extended Multiplicative Signal Correction
- 16:20 - 16:30 **Ilaria Idini** (Didcot, U.K.)
Changing the Face of Clinical Diagnostics Using Fourier Transform
Infrared (FTIR) Spectroscopy
- 16:35 - 16:45 **Mustafa Kansiz** (Melbourne, Australia)
Life Science Applications Using Novel Submicron Simultaneous IR &
Raman Microscopy – A New Paradigm in Vibrational Spectroscopy
- 16:50 - 17:00 **Matthias Godejohann** (Martinsried, Germany)
QCL-Based IR Microscopy: The Power of Real-Time Chemical Imaging
- 17:15 - 19:00 **Poster Session**

Poster Session

- P1 M. Darvin** (Berlin, Germany)
Application of Raman Microscopy in Analysis of Barrier-Related Parameters of Human
Stratum Corneum *in vivo*
- P2 C. Sandt** (Gifsur Yvette, France)
QUASAR
Intuitive Machine Learning Software for Spectroscopic Data
- P3 S. Delbeck, H.M. Heise**, (Iserlohn, Germany)
Monitoring of the Insulin-Dependent Glucose Metabolism of Human Monocytes in Cell
Cultures by Microdialysis and Infrared Spectrometry
- P4 Ch. Wichmann** (Berlin, Germany)
Is Freezing of Bacterial Samples the Way to Go?
- P5 R. Guliev** (Moscow, Russia)
The Use of FTIR for Reliable Bacterium Identification
- P6 C. Beleites** (Wölfersheim, Germany)
Cross-Validation Revisited: Using Uncertainty Estimates to Improve Model Autotuning
- P7 O. Bozkurt-Girit** (Ankara, Turkey)
Characteristics and Fiber Type Specific Distribution of Lipids in Skeletal Muscles of
Berlin Fat Mice Inbred (BFMI) Lines
- P8 Z. Heiner, F. Yesudas** (Berlin, Germany)
Probing One- and Two-Component Lipid Monolayers by Nonlinear Vibrational
Spectroscopy

- P9 A. Banas** (Singapore, Singapore)
Characterization of Compositional Changes in Fluoride- and Laser-Treated Enamel Caries Lesion
- P10 S. Garip Ustaoglu** (Istanbul, Turkey)
Application of Fourier Transform Infrared (FTIR) Microspectroscopy for the Assessment of Bone Quality
- P11 S. Vogt** (Tübingen, Germany)
Comparison of Fourier-Transform Infrared Spectroscopy and Whole Genome Sequencing for Strain Typing of *Enterobacter cloacae* Complex
- P12 T. Grunert** (Vienna, Austria)
Molecular Signatures of Fresh and Frozen/thawed Poultry Meat – Meat Authenticity Testing Using Machine Learning Assisted FTIR Spectroscopy
- P13 A. Nakar** (Jena, Germany)
Differentiation of *Enterobacteriaceae* using Single Cell Raman Spectroscopy
- P14 J. Waeytens** (Lillois, Belgium)
Investigation of Single Amyloids Fibrils at the Nanoscale: Challenges and Prospects using IR Nanospectroscopy AFMIR
- P15 P. Mamaeva** (Moscow, Russia)
ATR-FTIR Spectroscopy to Study Interaction of Mannose-Modified Polymers and Liposomes with Lectins
- P16 M. Pucetaite** (Lund, Sweden)
Sub-Micrometer Infrared Spectroscopy of Soil Fungal Exudates
- P17 C. Paluszkiwicz** (Krakow, Poland)
Examination of Selected Body Fluids Using Vibrational Spectroscopy
- P18 W. M. Kwiatek** (Krakow, Poland)
Investigation of Pathological Tissues Using Nanoscale Spectroscopy
- P20 G. Azemtsop Matanfack** (Jena, Germany)
Probing the Metabolic Activity State and the Functions of Single Heterotrophic Bacterial Cells via Raman Microspectroscopy and Stable Isotope Labeling
- P21 M. Grube** (Riga, Latvia)
Evaluation of Interactions Between DNA and Salts of 1,4-Dihydropyridine AV-153 by FTIR Spectroscopy
- P22 M.A.B. Hedegaard, S. V. Pedersen** (Odense, Denmark)
Forward Scattered Raman-Computed Tomography for 3D Imaging
- P23 H. Shen** (Jena, Germany)
Photonics as a Non-Destructive Investigation Strategy for Biofilms
- P24 B. Lorenz** (Jena, Germany)
Screening of *E. coli* Pathogenicity by Raman Microspectroscopy
- P25 F. Madzharova** (Berlin, Germany)
Multimodal Two-Photon Biospectroscopy Using Composite Plasmonic-BaTiO₃ Nanoprobes

- P26 G. P. Szekeres, C. Spedalieri** (Berlin, Germany)
Biocompatible Nanostructures for Label-Free SERS in Living Cells
- P27 N. Unger** (Jena, Germany)
Intracellular Raman Micro Spectroscopic Detection of Spectral Characteristics of *Chlamydia abortus* in Infected Buffalo Green Monkey Cells
- P28 F. Severcan** (Istanbul, Turkey)
Infrared Spectroscopy is a Promising Method in Disease Diagnosis from Body Fluids
- P29 M. Severcan** (Istanbul, Turkey)
Discrimination of Acutely and Gradually Heavy Metal (Cd or Pb) Acclimated Fresh Water Bacteria by FTIR Spectroscopy Coupled with Chemometrics
- P30 T. Lindtner, V. M. Rodriguez Zancajo** (Berlin, Germany)
FTIR Microspectroscopy of Organic and Inorganic Components of Plant Cells
- P31 A. R. Walther** (Odense, Denmark)
Fiber-optic Volume Probe for Subsurface Raman Spectroscopy in Turbid Media
- P32 A. Dogan** (Istanbul, Turkey)
Adipose Tissue in Inappropriate Lipid Storage
- P33 A. Pistiki** (Jena, Germany)
UV-Resonance Raman Spectroscopy of Inactivated Bacterial Pathogens for Determination of Resistance to β -Lactams and Carbapenems
- P34 S. Eiserloh** (Jena, Germany)
Visualizing an Intracellular Infection of Buffalo Green Monkey Cells by *Coxiella burnetii* with Raman Micro-Spectroscopy
- P35 S. Diehn** (Berlin, Germany)
Identification of Grass Pollen Species Using FTIR Microspectroscopy on Embedded Pollen Grains
- P36 Karlis Shvirksts** (Riga, Latvia)
FTIR Spectroscopy as a Tool for Basic Yeast Physiology Assessment
- P37 M. Lassen, H. Kerdoncuff** (Hørsholm, Denmark)
Sub-Shot Noise Coherent Raman Spectroscopy for Bio-optical Applications
- P38 C. Whitley** (Liverpool, U.K.)
New Statistical Algorithms and Scanning Methods for the Early Diagnosis of Cancer
- P39 D. E. Bedolla** (Clayton, Australia)
A Combined Study on the Damage by Soft X-Rays on Ultralene, Paraffin and on Paraffin-Embedded Fixed Tissues Using FTIR Spectroscopy and X-Ray Fluorescence.

Friday, October 11, 2019

Session chair: Janina Kneipp

- 09:00 - 09:20 **Monika Ehling-Schulz** (Vienna, Austria)
Differential Diagnostics of *Bacillus cereus* Group Members via Machine Learning Based FTIR Spectroscopy
- 09:25 - 09:45 **Jörg Rau** (Waiblingen, Germany)
MALDI-TOF MS and FT-IR Spectroscopy for Potentially Diphtheria-causing *Corynebacteria* – Cases and Applications
- 09:50 - 10:10 **Angela Novais** (Porto, Portugal)
At the Front Line of *Klebsiella pneumoniae* Capsular Polysaccharides Knowledge: FT-IR Spectroscopy as a Cost-effective Strain Typing Tool
- 10:15 - 10:30 **Petra Rösch** (Jena, Germany)
The Application of Different Raman Spectroscopic Techniques on Bacterial Samples
- 10:35 - 11:05 **Coffee Break**
- Session chair:** Richard A. Dluhy
- 11:05 - 11:25 **Norman Mauder** (Bremen, Germany)
The Bruker IR Biotyper. Development from Concept to Solution
- 11:30 - 11:50 **Ashraf Ismail** (Montreal, Canada)
Implementation of the New Generation of Compact ATR-FTIR Spectrometers for Microbial Identification and Typing in Clinical Settings
- 11:55 - 12:10 **Ariane Deniset-Besseau** (Orsay, France)
Chemical Speciation of Abnormal Deposits in Kidney Biopsy Using Infrared Nanospectroscopy AFMIR
- 12:15 - 12:30 **Luca Quaroni** (Krakow, Poland)
Nanoscale Infrared Measurements of Intact Eukaryotic Cells
- 12:35 - 12:50 **Oxana Klementieva** (Lund, Sweden)
New Light on Alzheimer's Disease: Novel Infrared Nanoimaging of Amyloid Beta-sheet Structures Directly in the Neurons
- 12:55 - 13:55 **Lunch**

Session chair: Peter Gardner

- 13:55 - 14:10 **Michael C. Martin** (Berkeley, USA)
Brain Cell Phenotyping by Infrared Spectroscopy
- 14:15 - 14:30 **Janina Kneipp** (Berlin, Germany)
SERS of Cells and of Pure Molecules (Nothing Compares)
- 14:35 - 14:50 **Mark Tobin** (Melbourne, Australia)
FTIR Microspectroscopy of Secondary Mineralization in EphrinB2-
Deficient Mice Displaying Brittle Bone Phenotype
- 14:55 - 15:20 **Coffee Break**

Session chair: Jürgen Schmitt

- 15:20 - 15:35 **Kamilla Malek** (Krakow, Poland)
Eosinophils and Neutrophils – A Combination of Raman and
Fluorescence Microscopy to Determine their Molecular Differences
- 16:40 - 16:00 **Max Diem** (Boston, USA)
Infrared Spectral Detection and Classification of Macrophage
- 16:00 16:10 **Final Discussion, Concluding Remarks**

Aim

The 2019 Workshop will continue the tradition of highlighting every two years the relevant fields of applications of biomedical vibrational spectroscopy and will bring together scientists using infrared and Raman spectroscopic techniques for the characterization and differentiation of intact microbial, plant, animal or human cells to promote exchange of ideas, experiences, and practical problem solutions. Following the lines of our last workshops in Berlin, major points of discussion will be the progress in vibrational spectroscopic research, recent applications in various fields of microbiology, bio-medicine and new technological developments.

Organization

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Sponsoring

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