



Workshop

FTIR Spectroscopy in Microbiological and Medical Diagnostics

Robert Koch-Institute, Berlin
October 19-20, 2017

Venue and Time

Robert Koch-Institute
Nordufer 20, 13353 Berlin, Germany

Registration: October 19, 2017 8:30 – 9:30
Beginning: October 19, 2017 9:30
Ending: October 20, 2017 16:55

Programme

Thursday, October 19, 2017

09:30 - 09:40 **Lothar H. Wieler** (President of the RKI)
Opening remarks

Session chair: **Janina Kneipp**

09:40 - 10:00 **Bayden R. Wood** (Clayton, Australia)
A new infrared spectroscopic point-of-care diagnostic for the detection and quantification of pathogens in red blood cells

- 10:05 - 10:25 **Howbeer Muhamadali** (Manchester, U.K.)
Quantitative differentiation of isotopically labelled *Escherichia coli* at single cell and community levels via multiple spectroscopy techniques
- 10:30 - 10:50 **Jörg Rau** (Stuttgart, Germany)
MALDI-TOF MS and FTIR spectroscopy for the identification and characterization of bacteria isolated from elephant and rhinoceros
- 10:55 - 11:25 **Coffee Break**
- Session chair: **Malgorzata Baranska**
- 11:25 - 11:45 **Ganesh D. Sockalingum** (Reims, France)
Identification of filamentous fungi by high-throughput FTIR spectroscopy and supervised chemometric methods
- 11:50 - 12:10 **Christoph Krafft** (Jena, Germany)
Towards translation of Raman spectroscopy for cell identification into clinical laboratories
- 12:15 - 12:35 **Janina Kneipp** (Berlin, Germany)
Multiphoton excitation and vibrational microspectroscopy of plant tissues
- 12:40 - 12:55 **Volha Shapaval** (Ås, Norway)
FTIR spectroscopy for analyzing lipids in microbial cells
- 13:00 - 14:10 **Lunch**
- Session chair: **Ganesh Sockalingum**
- 14:10 - 14:30 **Philip N. Bartlett** (Southampton, U.K.)
DNA detection and discrimination using electrochemical SERS
- 14:35 - 14:55 **Phil Heraud** (Clayton, Australia)
Infrared spectroscopy provides new insights in marine science
- 15:00 - 15:20 **Jean-Pierre de Vera** (Berlin, Germany)
Raman-spectroscopy for life detection on Mars and the Icy Moons in the outer solar system
- 15:25 - 15:45 **Giovanni Longo** (Rome, Italy)
Movement at the nanoscale to tackle biomedical challenges
- 15:50 - 16:20 **Coffee Break**

Session chair: **Jürgen Schmitt**

- 16:20 - 16:40 **Monika Ehling-Schulz** (Vienna, Austria)
FTIR spectroscopy – Biophotonics meets veterinary medicine
- 16:45 - 17:00 **Kamilla Malek** (Krakow, Poland)
FTIR spectroscopic imaging using standard and high magnification resolution: to detect inflamed and cancer cells *in vitro* and *ex vivo*
- 17:05 - 17:10 **Miriam Unger** (Santa Barbara, USA)
Latest advancements in nanoscale IR spectroscopy: spatial resolution, speed and spectral range
- 17:10 - 17:20 **Max Eisele** (Martinsried, Germany)
Exploring micro and nanobiological tissue at the nanoscale using infrared nano-spectroscopy (nano-FTIR)
- 17:20 - 17:30 **Markus Mangold** (Zurich, Switzerland)
Single-shot microsecond-resolved spectroscopy of the bacteriorhodopsin photo cycle with quantum cascade laser frequency combs
- 17:30 - 17:40 **Otto Hertzberg & Alexander Bauer** (Frankfurt/Main, Germany)
Mid-IR photothermal deflection spectrometer based on quantum cascade lasers: towards non-invasive glucose measurement
- 17:40 - 19:30 **Poster Session**

Poster Session

- P1 A. Banas** (Singapore, Singapore)
Qualitative analysis of human sebum in sebaceous glands in-situ using FTIR microspectroscopy
- P2 K. Banas** (Singapore, Singapore)
Comparison of work-flows for spectral data pre-processing and multivariate statistical analysis by means of open source solutions: orange (Python) and R studio (R language)
- P3 G. Bellisola** (Frascati, Italy)
Infrared analysis of cystic fibrosis (CF) cell models
- P4 O. Bibikova** (Berlin, Germany)
MIR-fiber spectroscopy for tumor sensing: in competition with Raman, NIR-reflection, fluorescence – or in combination?
- P5 R. Breitenbach, N. Knabe** (Berlin, Germany)
Microscopy-based Raman spectroscopy of fungal melanins in a genetically amenable *Ascomycete*
- P6 D. Casagrande Pierantoni** (Perugia, Italy)
High-contrast Brillouin and Raman micro-spectroscopy for simultaneous mechanical and chemical investigation of microbial biofilms

- P7 N. Chaudhary** (Dublin, Ireland)
Evaluation of T-cell activation with Raman microspectroscopy
- P8 E. Cordero** (Jena, Germany)
A compact Raman imaging system for bladder tissue analysis
- P9 L. Corte** (Perugia, Italy)
Merging FTIR and NGS for simultaneous phenotypic and genotypic identification of pathogenic *Candida* species
- P10 M. Dahms** (Jena, Germany)
Raman micro-spectroscopic identification of *Streptococcus pneumoniae* differentiated from other *Streptococcus* species
- P11 J. Denbigh** (Manchester, U.K.)
Synchrotron infrared microspectroscopy as a tool for probing drug-cell interactions in living biological cells
- P12 D. Fioretto** (Perugia, Italy)
Microbial single cell detection with Raman spectroscopy: taxonomic resolution and data accuracy
- P13 A. Flack** (Reims, France)
Vibrational spectroscopy as a high throughput technique for bacteria identification
- P14 S. Fornasaro** (Trieste, Italy)
Surface-enhanced Raman spectroscopy for therapeutic drug monitoring in oncology: a study on sample preparation
- P15 C. García-Timmermans** (Ghent, Belgium)
Sample preparation for bacteria identification with Raman spectroscopy
- P16 M. Grube** (Riga, Latvia)
FT-IR microspectroscopy of cancer cells and extracellular vesicles
- P17 T. Grunert** (Vienna, Austria)
Deciphering *Staphylococcus aureus* surface glycostructures by FTIR spectroscopy
- P18 C. Hartmann** (Munich, Germany)
Modified protein complexes for non-invasive molecular control
- P19 Z. Heiner** (Berlin, Germany)
Surface enhanced hyper Raman spectroscopy for bioapplications
- P20 H. M. Heise** (Iserlohn, Germany)
Silver halide fibers and other materials relevant for attenuated total reflection and transmission infrared spectroscopy: biocompatibility and toxicity testing using fibroblast cells
- P21 M. Hermes** (Exeter, U.K.)
Developing a rapid screening mid-IR imaging method for diagnosis of oesophageal cancer
- P22 P. Hoffmann** (Jena, Germany)
Detection of the cellular uptake and localization of photoCORMs by means of FT-IR micro-spectroscopic imaging

- P23 A. Jaworska** (Warsaw, Poland)
PM-IRRAS and AFM studies on modified ssDNA adsorbed on gold
- P24 K. Kochan** (Clayton, Australia)
AFM-IR nanoscale study of cell walls in living bacteria
- P25 C. Kratz** (Berlin, Germany)
Optofluidic platform for enhanced IR microscopic biosensing
- P26 F. Küçük Baloğlu** (Ankara, Turkey)
Investigation of therapeutic effect of palmitoleic acid on obesity induced type 2 diabetes in adipose tissue by Fourier transform infrared microspectroscopy
- P27 W. M. Kwiatek** (Kraków, Poland)
Application of AFM-IR to study human lenses and chromosomes
- P28 F. Lauer** (Berlin, Germany)
Identification of pollen grains in mixtures using hyperspectral MALDI-TOF MS imaging
- P29 I. M. Le-Deygen** (Moscow, Russia)
Interaction of magnetic nanorods coated by dopamine with anionic liposomes as revealed by FTIR spectroscopy
- P30 C. A. Lima** (São Paulo, Brazil)
Infrared spectroscopy determining the biochemical changes in premalignant skin lesions submitted to photodynamic therapy
- P31 X.-Y. Liu** (Jena, Germany)
Confocal Raman imaging integrated with non-negative matrix factorization analysis on spatiotemporal distribution of major components in biofilm
- P32 B. Lorenz** (Jena, Germany)
Preparation of blood samples for Raman microspectroscopy on single bacteria cells
- P33 J. Mathurin** (Orsay, France)
Label-free imaging to characterize new antibiotics carriers by IR nanospectroscopy
- P34 A. S. Mondol** (Jena, Germany)
Development of Raman platform for single cell analysis
- P35 O. Morgaienko** (Munich, Germany)
Visualization of pollutant degrading bacteria via bioorthogonal noncanonical amino acid tagging coupled to surface-enhanced Raman scattering
- P36 C. Paluszkiwicz** (Kraków, Poland)
Studies of cancerous tissues composition using FTIR and Raman microspectroscopy methods
- P37 L. Quaroni** (Kraków, Poland)
AFM-IR spectromicroscopy and imaging of vesicles, micelles, organelles and cytoskeletal structures in fibroblasts
- P38 L. Quaroni** (Kraków, Poland)
Nanoscale mid-infrared spectroscopic and imaging studies of single phospholipid bilayers as models of biological membranes

- P39 L. Roscini** (Perugia, Italy)
"Checker-FTIR": applying FTIR to checker board assays for drug mixtures inhibition tests
- P40 A. R  ther** (Clayton, Australia)
A multimodel approach to *Babesia bovis* diagnosis
- P41 I. W. Schie** (Jena, Germany)
High-throughput Raman spectroscopy of single cells
- P42 V. Shapaval** ( s, Norway)
FTIR spectroscopy for HT-screening and monitoring of single cell oil production
- P43 T. Shaykhtudinov** (Berlin, Germany)
IR nanopolarimetry: anisotropy in biomolecular assemblies and thin biofilms
- P44 K. Shvirksts** (Riga, Latvia)
Single factor stress response studies of mcf-7 breast cancer cells by FTIR spectroscopy
- P45 J. Solheim** ( s, Norway)
Fast resonant Mie-scatter correction algorithm: parameter choice and validation
- P46 L. Sykora** (Munich, Germany)
ATR-FTIR microplate reader and micromachined ATR silicon crystals
- P47 R. Weiss** (Munich, Germany)
Raman microspectroscopy for non-invasive, three-dimensional analysis of biofilms
- P48 C. Wichmann** (Jena, Germany)
Influence of CO₂-concentration on Raman spectra of bacteria
- P49 W. Yang** (Jena, Germany)
Fiber optic probe-based Raman imaging using positional tracking
- P50 I. Zeise** (Berlin, Germany)
Analysis of plant tissues using vibrational and other spectroscopic methods and multivariate approaches
- P51 Vesna  ivanovi ** (Berlin, Germany)
Comprehensive vibrational characterization of the interaction of liposomes and gold nanoparticles
- P52 C. F goli** (LaPlata, Argentina)
Vibrational micro- and nanospectroscopy of *Burkholderia contaminans* biofilms
- P53 C. Beleites** (W lfersheim,, Germany)
Experimental designs for comparing variance contributions in nested data
- P54 A.R. Walther** (Odense, Denmark)
Investigating the uptake and response of hMSC cells exposed to Falcarindiol
- P56 S. Diehn** (Berlin, Germany)
Hierarchical classification of variations in grass pollen quality using MALDI-TOF MS

Friday, October 20, 2017

Session chair: **Achim Kohler**

- 09:00 - 09:20 **Michael Wagner** (Vienna, Austria)
Functional analyses and targeted single cell genomics of microbes by Raman microspectroscopy
- 09:25 - 09:45 **Matthew J. Baker** (Glasgow, U.K.)
Developing spectroscopic processes for the detection of bacteria: environmental, surface deposited and high throughput
- 09:50 - 10:10 **Richard A. Dluhy** (Birmingham, USA)
Direct characterization of stored red blood cells using Raman spectroscopy
- 10:15 - 10:35 **Luísa Peixe** (Porto, Portugal)
Application of FTIR and MALDI-TOF MS for bacterial typing: a current standpoint
- 10:40 - 11:10 **Coffee Break**

Session chair: **Max Diem**

- 11:10 - 11:30 **Malgorzata Baranska** (Kraków, Poland)
Primary cells vs. cell lines: *in vitro* experiments and spectroscopic analysis
- 11:35 - 11:50 **Helene Oberreuter** (Stuttgart, Germany)
Cross-border Salmonellosis outbreak linked to fresh sprouts
– analysis of *Salmonella bovismorbificans* isolates by FTIR-spectroscopy
- 11:55 - 12:15 **Ariane Deniset-Besseau** (Orsay, France)
Advanced IR nanospectroscopy to study lipids bodies in micro-organisms: toward a better understanding of metabolic pathways at stake
- 12:20 - 12:35 **Curtis Marcott** (Athens, USA)
Non-contact methodology for obtaining submicron IR spectra and images of cells and tissue
- 12:40 - 12:55 **Petra Rösch** (Jena, Germany)
Cultivation-free identification of lung bacteria by means of Raman spectroscopy

13:00 - 14:00 **Lunch**

Session chair: **Ariane Deniset-Besseau**

14:00 - 14:20 **Achim Kohler** (Ås, Norway)
Model-based pre-processing for estimating scattering and absorption in infrared spectroscopy

14:25 - 14:45 **Cecilia Figoli** (La Plata, Argentina)
Vibrational micro- and nanospectroscopy of *Burkholderia contaminans* biofilms

14:50 - 15:05 **N. P. Ivleva** (Munich, Germany)
Applicability of SERS in combination with stable isotope approach for characterization of microorganisms at single cell level

15:10 - 15:40 **Coffee Break**

Session chair: **Bayden Wood**

15:40 - 15:55 **Gianluigi Cardinali** (Perugia, Italy)
FT-IR applied to microbial identification and stress response quantification: a preliminary balance and new perspectives

16:00 - 16:15 **Michael Hermes** (Exeter, U.K.)
Advancing mid infrared imaging technology: the Mid-TECH project

16:20 - 16:40 **Max Diem** (Boston, USA)
Results from a large-scale lung cancer spectral histopathology (SHP) study

16:45 - 16:55 **Final Discussion, Concluding Remarks**

Aim

The 2017 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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