



Workshop

FTIR Spectroscopy in Microbiological and Medical Diagnostics

Robert Koch-Institute, Berlin
October 15-16, 2015

Venue and Time

Robert Koch-Institute
Nordufer 20, 13353 Berlin, Germany

Registration: October 15, 2015 8:30 – 9:30

Beginning: October 15, 2015 9:30

End: October 16, 2015 17:20

Program

Thursday, October 15, 2015

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

Session chair: Jürgen Schmitt

09:40 - 10:00 **Roy Goodacre** (Manchester, U.K.)

Sniffing out bacteria: non-invasive volatile organic compound analysis of patients with ventilator associated pneumonia

- 10:05 - 10:25 **Volha Shapaval** (Ås, Norway)
Semi-automated identification and tracing of food related microorganisms by FTIR spectroscopy
- 10:30 - 10:50 **Alejandra Bosch** (La Plata, Argentina)
Evaluation of the metabolomic fingerprint of human embryo-spent-culture media by FTIR spectroscopy: A non-invasive assessment of embryo for in vitro fertilization (IVF) technology
- 10:55 - 11:25 **Coffee Break**
- Session chair:** Phil Heraud
- 11:25 - 11:45 **Bayden R. Wood** (Clayton, Victoria, Australia)
Malaria diagnosis using ATR-FTIR spectroscopy
- 11:50 - 12:10 **Natalia P. Ivleva** (Munich, Germany)
Stable isotope (Resonance) Raman microspectroscopic and SERS analysis of single microbial cells
- 12:15 - 12:35 **H. Michael Heise** (Iserlohn, Germany)
Infrared spectroscopy for fast characterization of fungi important in hygiene and agricultural sciences using micro-techniques
- 12:40 - 13:00 **Malgorzata Baranska** (Kraków, Poland)
High resolution imaging of single cells: Raman, FTIR, AFM and SNOM
- 13:05 - 14:15 **Lunch**
- Session chair:** Mareike Wenning
- 14:15 - 14:35 **Curtis Marcott** (Athens, USA)
Looking inside single cells and tissue using nanoscale infrared spectroscopy
- 14:40 - 15:00 **Ariane Deniset-Besseau** (Orsay, France)
Resonance enhanced AFM-IR: On the way to single molecule
- 15:05 - 15:25 **Francesco Simone Ruggeri** (Lausanne, Switzerland)
New insights into individual amyloid aggregates structure by infrared nanospectroscopy
- 15:30 - 15:50 **Matthew J. Baker** (Glasgow, U.K.)
Investigating bacterial agents and human response to bacterial agents via IR spectroscopy
- 15:55 - 16:25 **Coffee Break**

Session chair: Max Diem

- 16:25 - 16:45 **Richard Dluhy** (Birmingham, USA)
Detection of mycoplasma with SERS. Current laboratory results and progress towards clinical applications
- 16:50 - 17:10 **Wei E. Huang** (Oxford, U.K.)
Label-free detection of single cell phenotype using Raman micro-spectroscopy
- 17:15 - 17:35 **Ute Neugebauer** (Jena, Germany)
Spectroscopic characterization of infections: identification, localization and antibiotic susceptibility of the pathogen
- 17:40 - 19:45 **Poster Session**
- 20:00 - ?? **Dinner buffet** (at the RKI canteen)

Poster Session

- P1 V. Artyushenko** (Berlin, Germany)
Molecular spectroscopy methods for kidney cancer diagnostics
- P2 O.D. Ayala** (Nashville, USA)
Raman microspectroscopy for discrimination of bacterial pathogens causing acute otitis media
- P3 A. Bauer** (Frankfurt/Main, Germany)
Mid-IR photoacoustic spectroscopy on different skin locations for non-invasive blood glucose measurements
- P4 C. Beleites** (Jena, Germany)
A new N-FINDR algorithm and the unimixR package for spectral unmixing
- P5 G. Bellisola** (Verona, Italy)
Phenotyping cystic fibrosis cells by microFTIR and Principal Component Analysis
- P6 A. Bonifacio** (Trieste, Italy)
Label-free surface-enhanced Raman spectroscopy of biofluids: Diagnostic applications in oncology
- P7 J. Brückner** (Dresden, Germany)
The influence of increased iron concentrations on the biosilica of the marine diatom *Stephanopyxis turris*
- P8 T. Büchner, D. Drescher** (Berlin, Germany)
Multimethod approach to understand SERS nanoprobe in cells
- P9 K. Bulat** (Kraków, Poland)
High resolution imaging of endothelial cells by scanning near-field optical microscopy (SNOM)
- P10 J. De Meutter** (Brussels, Belgium))
Infrared imaging of high density protein arrays

- P11 A. Dogan** (Ankara, Turkey)
FT-IR spectroscopy and multivariate analysis for the detection of irradiated hazelnut (*Corylus avellana* L.)
- P12 K. Forfang** (Ås, Norway)
Estimating the efficiency of fatty acid extraction from fungal biomass by FTIR spectroscopy
- P13 S. Fornasaro** (Trieste, Italy)
Feasibility of quantitative determination of methotrexate with surface-enhanced Raman spectroscopy and multivariate calibration analysis
- P14 E. Giorgini** (Ancona, Italy)
Vibrational mapping of sinonasal lesions by Fourier transform infrared imaging spectroscopy
- P15 M. Godejohann** (Utting/Ammersee, Germany)
QCL-based IR microscopy: The power of real-time chemical imaging
- P16 M. Grube** (Riga, Latvia)
Evaluation of cancer-derived exosomes by FT-IR spectroscopy
- P17 M. Gühlke** (Berlin, Germany)
Study of combined one- and two-photon excited SERS-nanosensors for bio-applications
- P18 M.A.B. Hedegaard** (Odense, Denmark)
Applying noise adjusted principal component analysis for noise reduction of Raman micro spectroscopic image datasets
- P19 M. Hermes** (Jena, Germany)
Evaluating modulated excitation and conventional methods for background correction in Raman microscopy
- P20 O. Hertzberg** (Frankfurt/Main, Germany)
Mid-IR photothermal deflection spectroscopy enhanced by total internal reflection for non-invasive glucose monitoring
- P21 M. Joester** (Berlin, Germany)
Raman micro-spectroscopy and multivariate statistics to study the influence of silica on germinating pollen grains
- P22 A. Kerstan** (Waldbronn, Germany)
Pushing the limits of biomedical and biological FTIR imaging
- P23 L. Köhler** (Dresden, Germany)
The effect of variable calcium concentrations in culture media on the diatom species *Stephanopyxis turris* and *Thalassiosira pseudonana*
- P24 T. Konevskikh** (Ås, Norway)
Estimating and correcting Mie scattering in single cell infrared microspectroscopy
- P25 G. Kosa** (Ås, Norway)
Micro-cultivation of oleaginous fungi and high-throughput estimation of fatty acid profiles by FT-IR spectroscopy

- P26 W.M. Kwiatek** (Kraków, Poland)
NanoIR as a new tool for spectroscopic imaging in biomedical studies
- P27 L. Lovergne** (Glasgow, U.K.)
Developing serum based infrared spectroscopic diagnostics: Optimising sample preparation and sampling mode
- P28 R. Lukacs** (Ås, Norway)
Recovery of IR absorbance spectra of spherically shaped biological systems
- P29 K. Majzner** (Kraków, Poland)
Raman microscopic studies on the impact of high glucose condition on the endothelial cells
- P30 K. Malek** (Kraków, Poland)
FTIR spectroscopy in recognition of lifestyle diseases: Studies on blood plasma of animal models
- P31 M. Mangold** (Zürich, Switzerland)
QCL frequency comb technology for mid-infrared sensing
- P32 A. Mignolet** (Brussels, Belgium)
Investigation of polyphenols anti-cancerous action according to their differential effects on breast cancer cell lines by FTIR spectroscopy
- P33 A. Niedermayr** (Munich, Germany)
IR-spectroscopy and multivariate data analysis in point of care testing
- P34 M.Z. Pacia** (Kraków, Poland)
Diabetes, hypertension and cancer metastasis-induced changes in endothelium studied with 3D Raman and AFM imaging
- P35 S. Pahlow** (Jena, Germany)
Isolation and enrichment of bacteria for subsequent Raman spectroscopic identification
- P36 C. Paluszkiwicz** (Kraków, Poland)
AFM-IR spectroscopy of human lens at the nanoscale range
- P37 C. Pickering** (Glasgow, U.K.)
Experimental design for bacterial identification using vibrational spectroscopy
- P38 K. Ramser** (Luleå, Sweden)
Latest news on the development of a stimulated holographic endoscopic Raman imaging technique for early detection of colorectal cancer
- P39 S. Sabbatini** (Ancona, Italy)
Thermal stress effects in tumoral epithelial cells: SR-IRMS analysis
- P40 C. Sandt** (Gif sur Yvette, France)
Identification of a hypoxic signature in glioblastoma cells at the cellular and subcellular levels by FTIR microspectroscopy
- P41 J. Segmehl** (Zürich, Switzerland)
Ultrastructural and chemical investigation of functionalized wood cell walls using Raman microscopy

- P42 S. Seifert** (Berlin, Germany)
Classification and identification of aqueous pollen extracts using SERS and artificial neural networks (ANN)
- P43 T. Shaykhutdinov** (Berlin, Germany)
AFM-IR nanospectroscopy of aggregated thin porphyrin films: Correlating morphology with intermolecular stacking
- P44 K. Shvirksts** (Riga, Latvia)
Human mesenchymal stem cell studies by FT-IR spectroscopy
- P45 O. Sire** (Vannes, France)
Easy sampling and analysis FT-IR system for medical and biological diagnostic and screening
- P46 M. Smolina** (Brussels, Belgium)
Spectral differentiation of breast cancer cell lines in 2D and 3D cultures by infrared imaging
- P47 V. Tafintseva** (Ås, Norway)
Sparse partial least squares discriminant analysis (PLSDA) for classification of microorganisms using FTIR spectroscopy
- P48 S. Vercellone** (Verona, Italy)
Testing drugs targeting basic defect in cystic fibrosis (CF) epithelial cell lines by FTIR analysis
- P49 Vinay Kumar B.N.** (Jena, Germany)
Demonstration of carbon catabolite repression in naphthalene degrading soil bacteria via Raman spectroscopy based stable isotope probing
- P50 I. Zeise** (Berlin, Germany)
Microspectroscopic Raman imaging of cucumber plant tissues

Friday, October 16, 2015

Session chair: Roy Goodacre

- 09:00 - 09:20 **Markus Kostrzewa** (Bremen, Germany)
MALDI-TOF MS in microbiology – Introduction of an innovative physical technology into diagnostics
- 09:25 - 09:45 **Mareike Wenning** (Freising, Germany)
Identification and differentiation of food-related bacteria: A comparison of FTIR spectroscopy and MALDI-TOF mass spectrometry
- 09:50 - 10:10 **Ângela Novais** (Porto, Portugal)
Going deep in the inter- and intraspecies differentiation of clinically

relevant bacteria by MALDI-ToF MS and FTIR

- 10:15 - 10:35 **Jörg Rau** (Fellbach, Germany)
MALDI-TOF MS and FT-IR for bacteria "from fish and chips"
- 10:40 - 11:10 **Coffee Break**
- Session chair:** Bayden Wood
- 11:10 - 11:30 **Werner Mäntele** (Frankfurt/Main, Germany)
Photoacoustic and photothermal infrared spectroscopy of skin:
Options for non-invasive glucose measurement
- 11:35 - 11:55 **Luca Quaroni** (Kraków, Poland)
Mid-infrared spectro-microscopy of living cells: Quantitative studies of
reactions and metabolic networks
- 12:00 - 12:20 **Tom Grunert** (Vienna, Austria)
FTIR spectroscopy in host – pathogen interaction
- 12:25 - 12:45 **Norman Mauder** (Bremen, Germany)
Typing of bacteria via FT-IR spectroscopy – a complement for species ID
by MALDI TOF MS?
- 12:50 - 14:00 **Lunch**
- Session chair:** Richard Dluhy
- 14:00 - 14:20 **Dirk Schulze-Makuch** (Berlin, Germany, Pullman, USA)
Applications of Raman spectroscopy to astrobiological investigations
- 14:25 - 14:45 **Janina Kneipp** (Berlin, Germany)
Extending the capabilities of SERS in studies of cells
- 14:50 - 15:10 **Phil Heraud** (Clayton, Victoria, Australia)
Infrared spectroscopy: A new technique to understand the drivers of
Southern Ocean primary productivity
- 15:15 - 15:45 **Coffee Break**
- Session chair:** Janina Kneipp
- 15:45 - 16:05 **Rainer Hillenbrand** (Donostia-San Sebastian, Bilbao, Spain)
Nano-FTIR spectroscopy of individual protein complexes
- 16:10 - 16:30 **Paul W. Bohn** (Notre Dame, USA)
Chemical communication in microbial communities probed by correlated
Raman and mass spectrometric imaging

- 16:35 - 16:55 **Max Diem** (Boston, USA)
Cancer screening via infrared spectral cytopathology (SCP): Results for the upper digestive tract
- 17:00 - 17:20 **Final Discussion, Concluding Remarks**

Aim

The 2015 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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