FTIR
Forum
FTIR Diagnostics

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 nanoprobes 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. Paluszkiewicz** (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)
Photoaccoustic 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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