Detailed program

Sunday		
11:00-20:00		**Registration**
11:30-17:15	**Room**	**Workshop Session**
11:30-13:30	A0-01	Workshop session 1 HORIBA/COMEF **Raman imaging: discover the easiest and the most accurate ways to characterize micro & nano-plastics. Combine its full power to all your microscope in your lab with correlative microscopy.**
13:30-15:30	A0-03	Workshop session 2 WITec Raman Workshop **New Perspectives in 3D Raman Imaging and Correlative Techniques**
13:30-15:30	A0-04	Workshop session 2 Photothermal: O-PTIR Workshop **Submicron IR and Simultaneous Raman Microscopy with Co-Located Fluorescence Imaging**
15:30-17:15	**A0-01**	**CLIRSPEC session |** Chairs: Peter Gardner, Hugh Byrne
17:00-17:30		**Coffee break**
17:30-19:30	**A0-01**	**Perspective Session** Chairs: Kamilla Malek, Małgorzata Baranska, Janina Kneipp, Katarzyna Majzner
17:30-17:55	A0-01	**Progress in infrared spectroscopy** Kathleen Gough[1] [1]University of Manitoba
18:05-18:30	A0-01	**Frontiers of Advanced Vibrational Spectroscopy: The Molecular Chirality Perspective** Laurence Nafie[1] [1]Syracuse University
18:40-19:05	A0-01	**Strategies and perspectives to investigate the heme-enzymatic mechanism by resonance Raman spectroscopy** Giulietta Smulevich[1] [1]Dipartimento di Chimica “Ugo Schiff” (DICUS), Università di Firenze
19:30-21:30		**Welcome Cocktail – Conference Venue**
8:45-9:00	**A0-01**	**Opening Ceremony**

Monday		
9:00-10:15	**A0-01**	**Plenary Session** Chairs: Bin Ren, Harumi Sato
9:00-9:30	A0-01	**Can attenuated total reflectance infra red spectroscopy (ATR-IR) be used with polarised light?** Alison Rodger[1], Paul Wormell[2], Jun Koshubu[3], Junya Kitamura[3], Akihiro Sato[3] [1]Macquarie University [2]Western Sydney University [3]Jasco International
9:40-10:10	A0-01	**In-Operando Magneto-Raman Study of Graphene in the Quantum Hall Regime** Angela Hight Walker[1] [1]National Institute of Standards and Technology (NIST)
10:15-10:45		**Coffee Break**
10:45-12:10		**SESSION 1**
	A1-01	***(B) Structure&dynamics of molecules*** Chair: Ewan Blanch
10:45-11:00		**Probing the active site structural changes in P450/P420 forms of CYP121** Piotr Mak[1] [1]Saint Louis University
11:05-11:20		**Insights into molecules structure and dynamics by multi-wavelengths UV Resonance Raman spectroscopy** Barbara Rossi[1] [1]Elettra Sincrotrone Trieste
11:25-11:35		**Detection, characterization, and differentiation of SHb and HbFeIII–SH adducts inside functional erythrocytes** Jakub Dybaś[1], Tetiana Stepanenko[2], Grzegorz Zajac[1], Katarzyna M. Marzec[3] [1]Jagiellonian University, Jagiellonian Centre for Experimental Therapeutics (JCET) [2]Solaris National Synchrotron Radiation Centre, Jagiellonian University [3]AGH University of Science and Technology 3. Mot, A. C., Puscas, C., Dorneanu, S. A., & Silaghi-Dumitrescu, R. (2019). EPR detection of sulfanyl radical during sulfhemoglobin formation – Influence of catalase. Free Radical Biology and Medicine, 137, 110–115.DOI: 10.1016/j.freeradbiomed.2019.04.034
11:40-11:50		**Revealing the problem of the effective charge of iron ion in oxy-haemoglobin molecule** Katarzyna Dziedzic-Kocurek[1], Jakub Dybaś[2], Jan Stanek[1] [1]Faculty of Physics, Astronomy and Applied Computer Science, M. Smoluchowski Institute of Physics, Jagiellonian University
11:55-12:05		**Understanding Hydrogenases by 2D-IR Spectroscopy and Vibrational Perturbation Theory** Marius Horch[1], Yvonne Rippers[1], Cornelius Bernitzky[1], Solomon Wrathall[2], Barbara Procacci[2], Janna Schoknecht[3], Claudia Schulz[3], Christian Lorent[3], Catharina Kulka-Peschke[3], James Birrell[4], Ingo Zebger[3], Gregory Greetham[5], Oliver Lenz[3], Neil Hunt[2] [1]Freie Universitaet Berlin [2]University of York [3]Technische Universitaet Berlin [4]University of Essex [5]Rutherford Appleton Laboratory
	A1-02	***(C) Spectroscopy in local fields*** Chair: Volker Deckert
10:45-11:00		**Probing protein conformations at the nanoscale by means of IR nanospectroscopy** Antonia Intze[1], Maria Eleonora Temperini[1], Raffaella Polito[2], Michele Ortolani[2], Valeria Giliberti[3] [1]1Istituto Italiano di Tecnologia, Center for Life Nano- and Neuro-Science [2]Department of Physics, Sapienza University of Rome [3]Istituto Italiano di Tecnologia, Center for Life Nano- and Neuro-Science
11:05-11:20		**Nanophotonic platforms for enhanced chirally sensitive vibrational spectroscopy** Malcolm Kadodwala[1] [1]University of Glasgow

11:25-11:35		**Viewing interfacial chemistry through a graphene window with broadband infrared nanospectroscopy** Hans Bechtel[1], Jonathan Larson[2], Xiao Zhao[3], Xin He[2], Dong Li[4], Behzad Rad[4], Chunsheng Yan[4], Paul Ashby[4], Stephanie Gilbert Corder[1], Robert Kostecki[2], Miquel Salmeron[4] [1]Advanced Light Source, Lawrence Berkeley National Laboratory [2]Energy Storage & Distributed Resources Division, Lawrence Berkeley National Laboratory [3]Materials Sciences Division, Lawrence Berkeley National Laboratory [4]Molecular Foundry, Lawrence Berkeley National Laboratory
11:40-11:50		**Comparison of resonant and non-resonant reporter for the selection of brightest gold nanoparticles for Surface-enhanced Raman spectroscopy.** Megha Mehta[1], William Skinner[1], Sara Mosca[2], Benjamin Gardner[1], Francesca Palombo[1], Pavel Matousek[2], Nicholas Stone[1] [1]University of Exeter [2]STFC Rutherford Appleton Laboratory
	A0-04	***(F) Advances in instrumentation*** Chair: Kerstin Ramser
10:45-11:00		**Comparison of ATR-FTIR and O-PTIR techniques at ISMI beamline for the characterisation of biological and cultural heritage samples** Krzysztof Banas[1], Agnieszka Banas[1], Mark Breese[1] [1]Singapore Synchrotron Light Source
11:05-11:20		**Emerging Trend in AFM-IR: Surface-sensitive mode to probe sample's very surface** Ariane Deniset-Besseau[1], Jérémie Mathurin[2], Alexandre Dazzi[1] [1]Institut de Chimie-Physique, Université Paris-Saclay [2]Institut de Chimie-Physique, CNRS
11:25-11:35		**SR-FTIR Imaging of Live Cells Using a Novel Demountable Flow System to Study Phospholipidosis** Ohood Alshareef[1], K.L Andrew Chan[1], Ben Forbes[1], Mohamed Alhnan[1], Gianfelice Cinque[2] [1]Institute of Pharmaceutical Sciences, King's College London [2]Diamond Light Source, Harwell Science and Innovation Campus
11:40-11:50		**Infrared spectroscopy at the user facility ELI Beamlines** Nils Lenngren[1], Mateusz Rebarz[1], Jakob Andreasson[1], Miroslav Kloz[1] [1]The Extreme Light Infrastructure ERIC
11:55-12:05		**Current status of Chemical Infrared Imaging (CIRI / SOLAIR) beamline in Solaris** Maciej Roman[1], Danuta Liberda[1], Paulina Koziol[1], Karolina Kosowska[1], Tomasz P. Wrobel[1] [1]SOLARIS National Synchrotron Radiation Centre, Jagiellonian University
	A0-03	***(G) Analytical applications*** Chair: Young Mee Jung
10:45-11:00		**SERS combined with chemometric analysis for detection and identification of microorganisms: viruses and bacteria.** Agnieszka Kamińska[1], Krzysztof Niciński[1], Sylwia Berus[1], Dorota Korsak[2], Tomasz Szymborski[1], Beata Młynarczyk-Bonikowska[3], Monika Adamczyk-Popławska[2], Evelin Witkowska[1] [1]Institute of Physical Chemistry, Polish Academy of Sciences [2]University of Warsaw, Faculty of Biology, Institute of Microbiology [3]Department of Dermatology and Venerology, Medical University of Warsaw
11:05-11:20		**SISSI-Bio: the multipurpose infrared laboratory at Elettra synchrotron facility** Lisa Vaccari[1], Giovanni Birarda[1], Federica Piccirilli[1], Diana Eva Bedolla[2], Chiaramaria Stani[3] [1]Elettra Sincrotrotrone Trieste [2]Area Science Park [3]CERIC-ERIC
11:25-11:35		**SERS-based detection schemes in complex biological matrices** Dana Cialla-May[1], Natalia E. Markina[2], Alexey V. Markin[2], Juergen Popp[1] [1]Leibniz Institute of Photonic Technology [2]Saratov State University
11:40-11:50		**Quantitative Raman Analysis of Carotenoid Protein Complexes in Aqueous Solution** Joy Udensi[1], Ekaterina Loskutova[1], James Loughman[1], Hugh Byrne[1] [1]Technological University Dublin
11:55-12:05		**Towards a SERS electronic nose: VOC and gas sensing** Elle Wyatt[1], Marika Niihori[1], Sarah Sibug-Torres[1], Rakesh Arul[1], David- Benjamin Grys[1], Bart De Nijs[1], Jeremy Baumberg[1] [1]University of Cambridge

12:10-13:10		**Lunch**
13:10-14:35		**SESSION 2**
	A1-01	***(B) Structure&dynamics of molecules*** Chair: Federica Piccirilli
13:10-13:25		**Electrostatic and electrodynamic fields in lipid bilayer membranes** Lauren Webb[1] [1]The University of Texas at Austin
13:30-13:45		**Probing protein structure on nanoparticle surfaces using theoretical and experimental sum frequency scattering spectroscopy** Tobias Weidner[1] [1]Department of Chemistry, Aarhus University, Denmark, email: weidner@chem.au.dk
13:50-14:00		**FTIR studies of mutual interaction in PLL-doped DPPC/DPPG membranes: a powerful insight by chemometric analysis** Paulina Trombik[1], Mirosław Czarnecki[1], Katarzyna Cieślik-Boczula[1] [1]Faculty of Chemistry, University of Wroclaw, F. Joliot-Curie 14, 50-383 Wroclaw
14:05-14:15		**Crystalline purines in microalgae: Surprising robustness of the biosynthesis of crystalline guanine in dinoflagellates** Peter Mojzeš[1], Maxim Bokov[1], Radek Bura[1], Jana Pilátová[2] [1]Charles University, Faculty of Mathematics and Physics, Institute of Physics [2]Charles University, Faculty of Science, Department of Experimental Plant Biology
	A1-02	***(C) Spectroscopy in local fields*** Chair: Agata Królikowska
13:10-13:25		**Surface-Enhanced Anti-Stokes Intensity Fluctuations at High Speed** Alexandre Brolo[1], Nathan Lindquist[2] [1]University of Victoria [2]Bethel University
13:30-13:45		**Spectrally Resolved Super-Resolution Surface Enhanced Raman Scattering Imaging** Zachary Schultz[1] [1]The Ohio State University
13:50-14:00		**Beyond the metal core: leveraging stabilizer-metal interactions for direct SERS detection** Chiara Deriu[1], Laura Fabris[1] [1]Politecnico di Torino
14:05-14:15		**Exploring and Optimizing Factors Influencing Surface-Enhanced Raman Scattering (SERS) Performance** Sylwester Gawinkowski[1] [1]Institute of Physical Chemistry, Polish Academy of Sciences
14:20-14:30		**In vivo Real-time Multiplex Detection of Plant Signalling Molecules Using Surface-Enhanced Raman Scattering Nanosensor** Won Ki Son[1] [1]Seoul National University
	A0-04	***(F) Advances in instrumentation*** Chair: Agnieszka Banas
13:10-13:20		**Dxcover® Platform: The next generation of ATR-FTIR spectroscopy** Holly Butler[1], Loren Christie[1], Matthew J. Baker[2] [1]Dxcover Ltd [2]School of Medicine, University of Central Lancashire
13:25-13:35		**Infrared nanoimaging and nanospectroscopy – emerging tools for physical and (bio)chemical nanoanalytics** Adrian Cernescu[1] [1]attocube systems AG
13:40-13:50		**Most recent advances of QCL-IR microspectroscopy** Matthias Godejohann[1] [1]MG Optical Solutions
13:55-14:05		**Widefield Super-Resolution IR Imaging with Fluorescence Enhanced Photothermal Infrared** Miriam Unger[1], Mustafa Kansiz[1] [1]Photothermal Spectroscopy Corp

14:10-14:20		**Nano-Sized and Wearable Raman Spectrometers: Towards Widespread of SERs and Vibrational Spectroscopy** William Terziyan[1], Daniel Lauriola[1], Chase Wang[1] [1]BaySpec, Inc.
	A0-03	***(G) Analytical applications*** Chair: Yaakov Tischler
13:10-13:20		**Correlation analysis of spectroscopic and biological features to follow mesenchymal stem cell differentiation** Karolina Augustyniak[1], Hubert Latka[1], Monika Lesniak[2], Jacek Z. Kubiak[2], Robert Zdanowski[2], Kamilla Malek[1] [1]Jagiellonian University, Department of Chemical Physics 2Military Institute of Medicine – National Research Institute, Laboratory of Molecular Oncology and Innovative Therapies
13:25-13:35		**Thriving Advantages of Drug Combination in Osteosarcoma Treatment – A Vibrational Microspectroscopy Study** Raquel C. Laginha[1], Jéssica D. Silva[1], Maria Paula M. Marques[1], Gianfelice Cinque[2], Luís A. E. Batista de Carvalho[1], Ana L.M. Batista de Carvalho[1] [1]Molecular Physical-Chemistry R&D Unit [2]Diamond Light Source
13:40-13:50		**ATR-FTIR spectroscopic study of cells from the human monocytic cell line MONO-MAC-6 with stimulation by insulin** H. Michael Heise[1], Jacinta Tomas Borges[1], Yannik Merx[1], Saskia Simon[1], Sandra Stoppelkamp[1] [1]SOUTH-WESTPHALIA UNIVERSITY OF APPLIED SCIENCES
13:55-14:05		**Shedding new light on the action of cisplatin, 5-fluorouracil, and 5-azacytidine on primary Oral Squamous Carcinoma Cells by Raman Microspectroscopy coupled with multivariate statistical analyses** Valentina Notarstefano[1], Alessia Belloni[1], Paolo Mariani[1], Elisabetta Giorgini[1], Hugh J. Byrne[2] [1]Marche Polytechnic University [2]Technological University Dublin
14:10-14:20		**Multimodal Spectroscopic Imaging (MALDI MSI vs Raman imaging / FTIR) in the analysis of the secondary metabolites** Mikolaj Krysa[1], Katarzyna Suśniak[2], Monika Szymańska-Chargot[3], Anna Sroka-Bartnicka[1] [1]Independent Unit of Spectroscopy and Chemical Imaging, Biomedical Faculty, Medical University of Lublin [2]1Independent Unit of Spectroscopy and Chemical Imaging, Biomedical Faculty, Medical University of Lublin; 2 Department of Genetics and Microbiology, Institute of Biological Sciences, Maria Curie-Sklodowska University [3]Institute of Agrophysics, Polish Academy of Sciences
14:25-14:35		**Spectroscopic analysis of cancer-derived small extracellular vesicles for in vitro cancer diagnosis** Yuling Wang[1], Wei Zhang[1] [1]Macquarie University
14:30-15:00		**Coffee Break**
15:00-16:15		**SESSION 3**
	A1-01	***(B) Structure&dynamics of molecules*** Chair: Piotr Mak
15:00-15:10		**In-cell IR Difference Spectroscopy as a Time-resolved Method to Study Proteins in Living Cells** Lukas Goett-Zink[1], Anna Toschke[1], Eileen Baum[1], Tilman Kottke[1] [1]Bielefeld University / Biophysical Chemistry and Diagnostics
15:15-15:25		Nanosecond time-resolved IR spectroscopy on proteins using quantum cascade laser setups Jessica Klocke[1], Tilman Kottke[1] [1]Biophysical Chemistry and Diagnostics, Bielefeld University
15:30-15:40		**Rapidly determining the 3D structure of proteins by Surface-enhanced Raman spectroscopy** Hao Ma[1], Bin Ren[1] [1]Xiamen University

15:45-15:55		**Decoding early signs of erythrocyte pathology through analysis of protein secondary structure alterations** Tetiana Stepanenko[1], Katarzyna Bułat[2], Natalia Wilkosz[2], Fatih C. Alcicek[3], Jakub Dybas[4], Katarzyna M. Marzec[5] [1]Jagiellonian University, National Synchrotron Radiation Centre SOLARIS [2]Łukasiewicz Research Network, Krakow Institute of Technology [3]Goethe University, Institute for Cardiovascular Physiology [4]Jagiellonian University, Jagiellonian Centre for Experimental Therapeutics (JCET) 5AGH University of Science and Technology, Faculty of Physics and Applied Computer Science, Department of Medical Physics and Biophysics
16:00-16:10		**Hydration Structure of Biomaterials Studied by Infrared Spectroscopy and Chemometrics** Shigeaki Morita[1] [1]Osaka Electro-Communication University
	A1-02	***(C) Spectroscopy in local fields*** Chair: Zachary Schultz
15:00-15:15		**In-situ study of nanocatalytic reactions using surface-enhanced Raman spectroscopy** Hua Zhang[1] [1]College of Materials Xiamen University"
15:20-15:35		**Precision reuseable flow SERS for Healthcare BioSensors 2.0** Jeremy Baumberg[1] [1]University of Cambridge
15:40-15:50		**Exciton-Phonon Coupling in MoSe2/WSe2 Heterobilayers Probed Using Resonant Raman Spectroscopy** Oisín Garrity[1], Thomas Brumme[2], Annika Bergmann[3], Tobias Korn[3], Patryk Kusch[1], Stephanie Reich[1] [1]Freie Universität Berlin [2]Technische Universität Dresden [3]Universität Rostock
15:55-16:05		**In-Situ Cost-effective Methods for Fabricating SERS Substrates using Polydopamine** Ahmed Mahmoud[1], Alexandra Teixeira[1], Maria Sousa-Silva[1], Sara Abalde-Cela[1], Lorena Diéguez[1] [1]The International Iberian Nanotechnology Laboratory (INL)
16:10-16:20		**Vanadium oxide nanoparticles as non-plasmonic platforms for surface-enhanced Raman spectroscopy** Eva Kočišová[1], Anna Kuzminova[2], Marek Procházka[1], Ondřej Kylián[2] [1]Institute of Physics, Faculty of Mathematics and Physics, Charles University [2]Department of Macromolecular Physics, Faculty of Mathematics and Physics, Charles University
	A0-04	***(F) Advances in instrumentation*** Chair: Holly Butler
15:00-15:15		**Through the looking glass: Raman imaging through the bottle** Kishan Dholakia[1] [1]University of Adelaide
15:20-15:35		**New Approaches for Raman Spectroscopic Imaging and High-Throughput Monitoring in Biomedical Applications** Torsten Frosch[1] [1]Technical University Darmstadt
15:40-15:50		**Mode Optimized Tip-Enhanced Raman Scattering** Tao Chen[1], Wei Wang[1], Volker Deckert[1] [1]Friedrich-Schiller University
15:55-16:05		**Electric-field-dependent infrared nanospectroscopy of PVDF with an atomic force microscope** Maria Eleonora Temperini[1], Valeria Giliberti[2], Tommaso Venanzi[2], Raffaella Polito[1], Antonia Intze[1], Michele Ortolani[1] [1]Sapienza University of Rome
16:10-16:20		**Detection of microplastics using optical manipulation techniques and Raman spectroscopy** Silvie Bernatová[1], Martin Kizovský[1], Antonino Foti[2], Maria Donato[2], Pavel Zemánek[1], Ota Samek[1], Onofrio Maragò[2], Jan Ježek[1], Pietro Gucciardi[2] [1]Institute of Scientific Instruments of the Czech Academy of Sciences [2]Istituto per Processi Chimico-Fisici – Consiglio Nazionale delle Ricerche

	A0-03	***(G) Analytical applications*** Chair: Cassio Lima
15:00-15:10		**Chemically-specific in situ coherent Raman imaging of liquid-liquid phase separation in the crystallization process of pharmaceutical solids** Alba Arbiol[1], Laurin Zöller[2], Teemu Tomberg[1], Jukka Saarinen[1], Tom Konings[1], Sara Carlert[3], Eva Karlsson[3], Anders Borde[2], Quentin Vicentini[2], Christoph Saal[3], Jennifer Dressman[2], Clare Strachan[1] [1]Division of Pharmaceutical Chemistry and Technology, Viikinkaari 5E, 00014 University of Helsinki, Finland [2]Fraunhofer Institute for Translational Medicine and Pharmacology ITMP, Germany [3]AstraZeneca R&D Mölndal, S-431 83 Mölndal, Sweden
15:15-15:25		**Spectral identification of therapeutic allergen products** Christian Ickes[1], Pirya Rani[2], Kristiyana Tsenova[3], Johanna Rost[1], Frank Führer[1], Detlef Bartel[1], Christel Kamp[1] [1]Paul-Ehrlich-Institut [2]Saarland University [3]Goethe University
15:30-15:40		**Raman-based Detection of Antibiotics and Metabolites in Pharmaceutical Formulations and Clinical-relevant Matrices** Chen Liu[1], Jürgen Popp[1], Dana Cialla-May[2] [1]Institute of Physical Chemistry (IPC) and Abbe Center of Photonics (ACP), Friedrich Schiller University Jena, Member of the Leibniz Centre for Photonics in Infection Research (LPI), Helmholtzweg 4, 07743 Jena, Germany [2]Leibniz Institute of Photonic Technology, Member of Leibniz Health Technologies, Member of the Leibniz Centre for Photonics in Infection Research (LPI), Albert-Einstein-Straße 9, 07745 Jena, Germany
15:45-15:55		**Insights into triglycerides removal: Study using FTIR and Raman imaging in flow and static conditions** Gunjan Tyagi[1], Zain Ahmed[1], Joao Cabral[1], Sergei Kazarian[1] [1]Imperial College London
16:05-16:15		**Rare earth-citrate complexes study using surface-enhanced Raman scattering spectra** Hao Jin[1], Tamitake Itoh[2], Yuko. S. Yamamoto[1] [1]School of Materials Science, Japan Advanced Institute of Science and Technology [2]Nano-Bioanalysis Research Group, Health Research Institute, National Institute of Advanced Industrial Science and Technology
16:30-18:45		**POSTER SESSION 1**
		Chairs: Lisa Vaccari, Shigeaki Morita
16:30-17:30	A0-01	Flash Presentations (Topics A-F, J)
17:30-18:45		Poster Session (Topics B-D)
18:00-18:45		**Steering Committee meeting**

Tuesday		
9:00-10:15	**A0-01**	**Plenary Session**
		Chair: Gulietta Smulevich
9:00-9:30		**What we learn with new time-resolved Raman spectrometers** Koichi Iwata[1] [1]Gakushuin University
		Chair: Yukihiro Ozaki
9:40-10:10		**Ultrafast Structural Dynamics in Various π-Conjugated Molecular Systems Probed by Time--resolved Electronic and Vibrational Spectroscopy** Dongho Kim[1] [1]Department of Chemistry, Yonsei University
10:15-10:45		**Coffe Break**
10:45-12:10		**SESSION 1**
	A1-01	***(B) Structure&dynamics of molecules*** Chair: Valeria Giliberti
10:45-11:00		**Domain movements and conformational changes in large membrane proteins identified by combined SEIRAS and IR labelling approach** Petra Hellwig[1], Tatjana Gerasimova[2], Ana Filipa Seica Santos[3], Thorsten Friedrich[4] [1]University of Strasbourg CNRS, UMR 7140 [2]University of Strasbourg and University of Freiburg [3]University of Strasbourg, UMR 7140 [4]University of Freiburg, Institute for Biochemistry
11:05-11:20		**Local Structural Dynamics of Membrane Protein Bacteriorhodopsin Revealed by 2D Vibrational Spectroscopy** Jianping Wang[1] [1]Institute of Chemistry
11:25-11:35		**Plasmonic infrared study of SARS COV-2 mPro dimerization and its inibition** Federica Piccirilli[1], Giovanni Birarda[1], Lisa Vaccari[1], Hendrik Vondracek[1], Lucia Silvestini[2], Francesco Spinozzi[3], Paolo Mariani[3], Antonio Palumbo Piccionello[4], Vincenzo Aglieri[5], Andrea Toma[5], Maria Grazia Ortore[3] [1]Elettra Sincrotrone Trieste [2]Università politecnica delle Marche [3]Università Politecnica delle Marche [4]Università degli studi di Palermo [5]Istituto Italiano di tecnologia
11:40-11:50		**The chemical structure and conformation of tau protein aggregates at the growth phase** Kamila Sofińska[1], Sara Seweryn[1], Katarzyna Skirlińska-Nosek[1], Piotr Batys[2], Jakub Barbasz[2], Ewelina Lipiec[1] [1]Jagiellonian University, Faculty of Physics, Astronomy, and Applied Computer Science, M. Smoluchowski Institute of Physics [2]Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences
	A1-02	***(C) Spectroscopy in local fields*** Chair: Eva Kočišová
10:45-11:00		**Studying Metal-Molecule Interactions to Improve SERS Sensor Performance** Laura Fabris[1], Chiara Deriu[1], Kaleigh Scher[2], Shaila Thakur[1] [1]Politecnico di Torino [2]Rutgers University
11:05-11:20		**Comparative study of p-Aminothiophenol adsorption by Surface-Enhanced Raman Spectroscopy** María Rosa López-Ramírez[1], María De la Cabeza Fernández[2], Alexis Alvear-Fernández[2], Rafael Contreras-Cáceres[3] [1]Department of Physical Chemistry, Faculty of Science, University of Málaga [2]Department of Chemistry in Pharmaceutical Sciences, Faculty of Pharmacy, Universidad Complutense de Madrid [3]Department of Chemistry and Physics, University of Almería

11:25-11:35		**Searching for one-armed thiol bandit – SERS and DFT studies on adsorption modes of cyclo(L--Cys-D-Cys) on silver** Agata Królikowska[1], Marcin Witkowski[1], Lasse Jensen[2], Wojciech Dzwolak[1] [1]Faculty of Chemistry, University of Warsaw, Pasteura 1 [2]Department of Chemistry, Penn State University, 101 Chemistry Building, University Park, 16802, PA
11:40-11:50		**A newly recognized chemically stable surface bound thiolate intermediate in plasmon-induced catalysis** Xiaobin Yao[1], Sadaf Ehtesabi[2], Christiane Höppener[1], Tanja Deckert-Gaudig[1], Henrik Schneidewind[3], Stephan Kupfer[2], Stefanie Gräfe[2], Volker Deckert[1] [1]1. Friedrich Schiller University Jena, Institute of Physical Chemistry and Abbe Center of Photonics, Helmholtzweg 4, Jena 07743, Germany; 2. Leibniz Institute of Photonic Technology, Albert-Einstein-Str.9, Jena 07745, Germany [2]1. Friedrich Schiller University Jena, Institute of Physical Chemistry and Abbe Center of Photonics, Helmholtzweg 4, Jena 07743, Germany [3]2. Leibniz Institute of Photonic Technology, Albert-Einstein-Str.9, Jena 07745, Germany
11:55-12:05		**Pushing the limits of Raman Spectroscopy: Photo-induced enhanced Raman Spectroscopy on Ag-TiO2 hybrid nanoplatforms** Łukasz Pięta[1], Aneta Kisielewska[2], Ireneusz Piwoński[2], Kamilla Małek[1] [1]Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Krakow, Poland [2]Department of Materials Technology and Chemistry, Faculty of Chemistry, University of Lodz, Pomorska 163, 90-236 Lodz, Poland
	A0-04	***(F) Advances in instrumentation*** Chair: Wojciech Kwiatek
10:45-10:55		**Simultaneous SERS & SEIRA with Single Molecule Detection – The Application and Characterization of Plasmonically Resonant Structures with Sub-Micron Optical Photothermal Infrared and Simultaneous Raman spectroscopy** Mustafa Kansiz[1], Miriam Unger[2], Deepthy Kavungal[3], Felix Richter[4], Hatice Altug[3], Mark Anderson[5] [1]Photothermal Spectroscopy Corp [2]Photothermal Spectroscopy Corp GmbH [3]Bionanophotonic Systems (BIOS) Laboratory & Lashuel Lab, EFPL [4]Bionanophotonic Systems (BIOS) Laboratory & Lashuel Lab, EFPL, [5]Caltech, Jet Propulsion Labs, NASA
11:00-11:10		**Raman optical activity as a sensitive tool in analytical chemistry** Josef Kapitán[1], Pavel Michal[1], Jana Hudecová[1], Petr Bouř[2] [1]Palacký University Olomouc, Department of Optics [2]Institute of Organic Chemistry and Biochemistry, Academy of Sciences
11:15-11:25		**A novel wide-field Raman imaging setup** B. J. A Mooij[1], R. W. Schmidt[1], W. A. J. Vijvers[2], F. Ariese[1] [1]LaserLaB, Vrije Universiteit Amsterdam [2]Chromodynamics B.V.
11:30-11:40		**Simultaneous co-located Raman and SEM imaging for correlated SEM microscopy** Jorge Diniz[1], Agnieszka Sozanska[2], Tim Batten[3] [1]Renishaw plc [2]Renishaw Spzoo [3]Renishaw PLC
11:45-11:55		**Reducing frequency fluctuations induced by back-reflected light into a non-stabilized low cost laser diode** Konstantinos Stergiou[1], Oleksii Ilchenko[2], Yurii Pilhun[1], Andrii Kutsyk[2] [1]Lightnovo ApS [2]Technical University of Denmark
12:00-12:10		**Maximizing Positive Microplastic Particle Identification and Provenance Through Optimized Optical and Raman Microscopy – Particle-Correlated Raman Spectroscopy (PCRS)** Andrew Whitley[1], Eunah Lee[1], Massimiliano Rocchia[1], Sebastien Laden[1] [1]HORIBA
	A0-03	***(G) Analytical applications*** Chair: Entesar Al-Hetlani

10:45-10:55		**Silicon within fossil and cultivated coccoliths of Helicosphaera carteri: new insights from Infrared Spectromicroscopy and X-ray Fluorescence analyses** Giovanni Birarda[1], Manuela Bordiga[2], Diana Eva Bedolla[3], Alessandra Gianoncelli[1], Simone Pollastri[1], Valentina Bonanni[1], Gianluca Gariani[1], Lisa Vaccari[1], Federica Cerino[2], Marina Cabrini[2], Alfred Beran[2], Mario Zanoni[4], Maurizio Zuccotti[4], Giulia Fiorentino[4], Miriam Cobianchi[5], Andrea Di Giulio[5], Claudia Lupi[5] [1]Elettra—Sincrotrone Trieste [2]National Institute of Oceanography and Applied Geophysics OGS [3]AREA Science Park [4]Department of Biology and Biotechnologies "Lazzaro Spallanzani", University of Pavia [5]Department of Earth and Environmental Sciences, University of Pavia
11:00-11:10		**Methods of vibrational microspectroscopy for the assessment of the internalization, biodistribution, fate and toxicity of nano- and microparticles at in vitro and in vivo conditions** Joanna Chwiej[1], Natalia Janik-Olchawa[2], Agnieszka Dróżdż[3], Aleksandra Wajda[2], Maciej Sitarz[1], Daniel Horak[4], Michal Babic[4], Jolanta Gol[1], Zuzanna Setkowicz-Janeczko[2], Aleksandra Wilk[1], Marzena Rugieł[1], Katarzyna Matusiak[1], Christoph Sandt[5], Ferenc Borondics[5], Magdalena Wytrwał-Sarna[1] 1AGH University of Krakow [2]Jagiellonian University [3]Maria Curie-Skłodowska University in Lublin [4]Czech Academy of Sciences [5]SOLEIL
11:15-11:25		**The increase of fibres and flavonoids concentration in the Zea mays stem treated with Nod-factor-based biofertilizer. A multimodal imaging study.** Mikolaj Krysa[1], Katarzyna Susniak[2], Cai Li Song[3], Monika Szymanska-Chargot[4], Artur Zdunek[4], Izabela S. Pieta[5], Janusz Podlesny[6], Anna Sroka-Barnicka[1], Sergei G. Kazarian[3] [1]Medical University of Lublin, Independent Unit of Spectroscopy and Chemical Imaging, [2]Maria Curie-Sklodowska University, Department of Genetics and Microbiology [3]Imperial Collage London, Department of Chemical Engineering [4]Institute of Agrophysics, Polish Academy of Sciences [5]Institute of Physical Chemistry, Polish Academy of Sciences [6]Institute of Soil Science and Plant Cultivation, State Research Institute
11:30-11:40		**Development of Raman Spectroscopic analysis techniques to assess quality biomarkers in fish** Jeremy Landry[1], Peter Torley[1], Ewan Blanch[1] [1]RMIT University
11:45-11:55		**Visualization and identification of components in a gigantic spherical dolomite concretion by Raman imaging and MCR analysis** Ryosuke Kitanaka[1], Motohiro Tsuboi[2], Tomoko Numata[3], Yusuke Muramiya[4], Hidekazu Yoshida[5], Yukihiro Ozaki[2] [1]Kewansei Gakuin University [2]Kwansei Gakuin University [3]HORIBA Techno Setvice Co. Ltd. [4]Fukada Geological Institute [5]Nagoya University
12:00-12:10		**SIP vibrational microspectroscopy in micro-structured chips reveals single-cell metabolic dynamics of soil microbes** Milda Pucetaite[1], Edith C. Hammer[1], Louise C. Andresen[2], Sofía Gabriela Rodas Samayoa[2] [1]Department of Biology, Lund University [2]Department of Earth Science, University of Gothenburg
	A0-01	***(H) Biodiagnostic spectroscopy*** Chair: Nick Stone

10:45-11:00		**High-resolution Raman imaging of >300 cells from human patients affected by nine different leukemia subtypes: a global clustering approach** Renzo Vanna[1], Andrea Masella[2], Manuela Bazzarelli[2], Paola Ronchi[3], Aufried Lenferink[4], Cristina Tresoldi[3], Carlo Morasso[5], Marzia Bedoni[6], Dario Polli[7], Fabio Ciceri[3], Giulia De Poli[2], Matteo Bregonzio[2], Cees Otto[4] [1]Istituto di Fotonica e Nanotecnologie – Consiglio Nazionale delle Ricerche (IFN-CNR) [2]3rdPlace SRL [3]IRCCS Ospedale San Raffaele [4]University of Twente [5]IRCCS Istituti Clinici Scientifici Maugeri [6]IRCCS Fondazione Don Carlo Gnocchi [7]Politecnico di Milano
11:05-11:20		**Surface Enhanced Spatially Offset Raman Spectroscopy: A Promising Optical Imaging Modality in Preclinical Cancer Imaging** Fay Nicolson[1], Eunah Lee[2], Andrew Whitely[2], Bohdan Andreiuk[3], Scott Rudder[4], Samuel Mabbott[5], Kevin Haigis[1] [1]Dana-Farber Cancer Institute [2]HORIBA Scientific [3]Dana-Farber Cancer Insitute [4]Opto-Sigma [5]Texas A&M University
11:25-11:35		**Surface-enhanced Raman Spectroscopy in tumor detection** Aneta Kowalska[1], Marta Czaplicka[1], Ariadna Nowicka[2], Tomasz Szymborski[3], Izabela Chmielewska[4], Wojciech Kukwa[5], Agnieszka Kamińska[3] [1]Institute of Physical Chemistry Polish Academy of Sciences [2]Institute for materials Research and Quantum Engineering, Poznań University [3]Institute of Physical Chemistry, Polish Academy of Sciences [4]Department of Pneumonology, Oncology and Allergology, Medical University of Lublin [5]Szpital Czerniakowski, Medical University of Warsaw
11:40-11:50		**FTIR Spectroscopy for Bladder Carcinoma Detection and Prediction of Grade, Invasion, and Lymph Nodes Metastases** Monika Kujdowicz[1], David Perez-Guaita[2], Piotr Chlosta[3], Krzysztof Okon[4], Kamilla Malek[5] [1]Department of Patomorphology, Jagiellonian University Medical College; Faculty of Chemistry, Jagiellonian University [2]Department of Analytical Chemistry, University of Valencia [3]Department of Urology, Jagiellonian University Medical College [4]Department of Patomorphology, Jagiellonian University Medical College [5]Faculty of Chemistry, Jagiellonian University
11:55-12:05		**Raman Spectroscopic application in cervical cancer screening** Rubina Shaikh[1], Aoife Mc Guinness[2], Alison Malkin[3], John O'Leary[4], Cara Martin[4], Fiona Lyng[2] [1]Marie Curie Fellow 1.Centre for Radiation and Environmental Science, FOCAS Research Institute, Technological University Dublin, Ireland. 2.School of Physics & Clinical & Optometric Sciences, Central Quad, Technological University Dublin – City Campus, Gr [2]1.Centre for Radiation and Environmental Science, FOCAS Research Institute, Technological University Dublin, Ireland. 2.School of Physics & Clinical & Optometric Sciences, Central Quad, Technological University Dublin – City Campus, Grangegorman, Ireland [3]TU Dublin [4]TCD CERVIVA Molecular Pathology Laboratory, The Coombe Women and Infants University Hospital, Dublin, Ireland.5. Trinity St James Cancer Institute, Trinity College Dublin, Ireland
12:10-13:10		**Lunch**
13:15-14:30		**POSTER SESSION 2**
		Poster Session (Topics A, E, F, J)
14:45-18:00		**Excursion**
19:00		**Beer Club**

Wednesday		
9:00-10:15		**Plenary Session**
		Chair: Kathleen Gough
9:00-9:30		**Advances and applications in FTIR spectroscopic imaging for studies of dynamic systems** Sergei Kazarian[1] [1]Imperial College London
		Chair: Christian Huck
9:40-10:10		**IR-control of ultrafast excited state dynamics in transition metal complexes** Topic: plenary and perspective lectures Julia Weinstein[1], Iona Ivalo[1], Rory Cowin[1], Martin Appleby[1], Catherine Royle[1], Igor Sazanovich[2], Dimitri Chekulaev[3], Anthony Meijer[1], Alexander Auty[1], Guaznhi Wu[1], Tao Cheng[1], James Shipp[1] [1]University of Sheffield [2]Central Laser Facility, Rutherford Appleton Laboratory [3]Lord Porter Laser Laboratory, University of Sheffield
10:15-10:45		**Coffee Break**
10:45-12:10		**SESSION 1**
	A1-01	***(B) Structure&dynamics of molecules*** Chair: Judith Mihály
10:45-10:55		**Raman Spectroscopic Investigations of the Mechanisms of Inhibition of Protein Fibrils by Novel Spirooxindole Compounds** Anthony Dahdah[1], Subashani Maniam[1], Nilamuni De Silva[1], Helmut Huegel[1], Ewan Blanch[1] [1]RMIT University
11:00-11:10		**State of water in various environments: aliphatic ketones. MIR/NIR spectroscopic, dielectric and theoretical studies** Mirosław Czarnecki[1], Krzysztof Beć[2], Justyna Grabska[2], Christian Huck[2], Sylwester Mazurek[1], Kazimierz Orzechowski[1] [1]University of Wrocław [2]University of Innsbruck
11:15-11:25		**Near-Infrared and visible excited Raman optical activity in the study of B12 derivatives: far-from--resonance vs strong resonance approach** Ewa Machalska[1], Grzegorz Zając[1], Monika Halat[2], Takumi Tani[3], Tomotsumi Fujisawa[3], Masashi Unno[3], Malgorzata Baranska[1] [1]Jagiellonian Centre for Experimental Therapeutics (JCET), Jagiellonian University [2]Department of Plant Biology and Biotechnology, Faculty of Biotechnology and Horticulture, University of Agriculture [3]Department of Chemistry and Applied Chemistry, Faculty of Science and Engineering, Saga University
11:30-11:40		**Evaluating the acidity levels in super-acidic ionic liquids by Raman Spectroscopy** Cedric Malherbe[1] [1]University of Liege
11:45-11:55		**Unraveling the Structural Polymorphism of Mononucleotide G-Quadruplexes via Raman Optical Activity** Štěpán Jílek[1], Josef Kapitán[2], Mohammed Siddique Para Kkadan[1], Ivan Barvík1, Václav Profant[1] [1]Institute of Physics, Faculty of Mathematics and Physics, Charles University [2]Department of Optics, Faculty of Science, Palacký University Olomouc
	A1-02	***(E) Nonlinear vibrational spectroscopy*** Chair: Freek Ariese
10:45-11:00		**Proteins at charged biointerfaces as revealed by nonlinear vibrational spectroscopy** Zsuzsanna Heiner[1] [1]Humboldt-Universität zu Berlin, SALSA
11:05-11:20		**Time-domain Raman spectroscopy for large-scale cell screening** Kotaro Hiramatsu[1] [1]The University of Tokyo

11:25-11:35		**Good vibrations: small molecule raman optical probes to image metabolism in tissue micro-environments** Ailsa Geddis[1], Fabio De Moliner[1], Colin Campbell[1], Marc Vendrell[1] [1]University of Edinburgh
11:40-11:50		**Probing amide I-water vibrational coupling in α-helical and β-strand protein structures with two-color two-dimensional infrared spectroscopy** Fani Madzharova[1], Adam Chatterley[1], Steven Roeters[1], Tobias Weidner[1] [1]Aarhus University
11:55-12:05		**Molecular structure, surface charge and dissolution of the MgO-water interface influenced by liquid flow** Moritz Zelenka[1], Ellen H. G. Backus[1] [1]University of Vienna
	A0-04	***(F) Advances in instrumentation*** Chair: Yusuke Morisawa
10:45-11:00		**New Perspectives for Mid-IR Spectroscopy of Liquids as Enabled by Quantum Cascade Lasers** Bernhard Lendl[1], Alicja Dabrowska[1], Daniel-ralph Hermann[1], Giovanna Ricchiuti[1], Gustavo Lukasievicz[1], Georg Ramer[1] [1]TU Wien
11:05-11:20		**Stimulated Raman scattering and resonance Raman spectroscopy combined with holography, interferometry and video imaging** Kerstin Ramser[1] [1]Department of Engineering Sciences and Mathematics/Luleå University of Technology
11:25-11:35		**Developing Sensitive Stimulated Raman Scattering (SRS) Microscopy** Krzysztof Brzozowski[1], Anna Pieczara[2], Malgorzata Baranska[3] [1]Jagiellonian University [2]Jagiellonian Centre for Experimental Therapeutics [3]Jagiellonian University, Jagiellonian Centre for Experimental Therapeutics
11:40-11:50		**Rapid field-resolved infrared fingerprinting and discrimination of particles in flow** Marinus Huber[1], Daniel Gerz[1], Holger Mirkes[2], Florian Lindinger[2], Yannick Münzenmaier[2], Alexander Weigel[3], Mark Kielpinski[1], Thomas Henkel[1], Mihaela Zigman[3], Ferenc Krausz[3], Jürgen Popp[1], Ioachim Pupeza[1] [1]Leibniz Institute of Photonic Technology [2]Ludwig Maximilians University [3]Max Planck Institute of Quantum Optics
11:55-12:05		**Current state of spectrometer miniaturization: synergy with analytical potential of NIR spectroscopy** Christian W. Huck[1], Justyna Grabska[1], Krzysztof B. Bec[1] [1]University of Innsbruck
	A0-03	***(G) Analytical applications*** Chair: Maria Lopez-Ramirez
10:45-11:00		**Probing chemical speciation with low-frequency Raman spectroscopy** Keith Gordon[1] [1]University of Otago and Dodd Walls Centre – Te Whai Ao
11:05-11:20		**Profiling of Human Bones by Vibrational Spectroscopy** Maria Paula Marques[1], David Gonçalves[2], Stewart F. Parker[3], Winfried Kockelmann[3], Giulia Festa[4], Luís Batista de Carvalho[1] [1]Univ. Coimbra, Molecular Physical-Chemistry R&D Unit [2]Archaeosciences Lab., Directorate General Cultural Heritage [3]ISIS Facility, STFC Rutherford Appleton Laboratory [4]CREF – Museo Storico della Fisica e Centro Studi e Ricerche Enrico Fermi

11:25-11:35		**Fusion of IR and RS spectral data in 2D and 3D in vitro studies for the spheroid blood-brain barrier model** Anna Antolak[1], Aleksandra Pragnąca[2], Zuzanna Krysiak[3], Monika Leśniak[3], Joanna Korszun[4], Robert Zdanowski[3], Kamilla Małek[1] [1]Jagiellonian University [2]Jagiellonian University, Doctoral School of Exact and Natural Sciences [3]Military Institute of Medicine National Research Institute [4]Military Institute of Medicine National Research Institute; Bio-Med-Chem Doctoral School of the University of Lodz and Lodz Institute of the Polish Academy of Sciences
11:40-11:50		**Aging in coronal dentine of the human tooth seen at the sub-micron resolution in non-contact IR spectroscopy** Agnieszka Banas[1], Krzysztof Banas[1], Chin-ying, Stephen Hsu[2], Guang Rong Tang[2], Mark B.H. Breese[1] [1]Singapore Synchrotron Light Source NUS [2]National University of Singapore, Dentistry Department
11:55-12:05		**Micro and nano-spectroscopic studies of modified metallic surface for implantology application** Dominika Święch[1], Gaetano Palumbo[1], Natalia Piergies[2], Kamila Kollbek[3], Czesława Paluszkiewicz[2] [1]AGH University of Science and Technology, Faculty of Foundry Engineering, av. Mickiewicza 30 [2]Institute of Nuclear Physics Polish Academy of Sciences [3]AGH University of Science and Technology, Academic Centre for Materials and Nanotechnology, av. Mickiewicza 30
	A0-01	***(H) Biodiagnostic spectroscopy*** Chair: Anna Sroka-Bartnicka
10:45-11:00		**Portable Raman spectroscopy for in-clinic skin and prostate cancer diagnosis** Suse J. Van Breugel[1], Hannah Matthews[1], Kamran Zargar-Shoshtari[2], Paul Jarret[3], Michelle Locke[4], Cather Simpson[1], Michel Nieuwoudt[1], Claude Aguergaray[1] [1]The University of Auckland [2]Counties Manukau District Health Board [3]Department of Dermatology, Middlemore Hospital [4]Department of Plastic Surgery, Middlemore Hospital
11:05-11:20		**Self-assembled nanogap arrays of gold nanoparticles in dimple nanopores induced by DNA hybridization** Hajun Dang1, Jaebum Choo[1] [1]Chung-Ang University
11:25-11:35		**An injectable biosensor for continuous remote monitoring of patients with prostate cancer** Marta Aranda Palomer[1], Maria S. Relvas[2], Sergio Quintero[1], Jason B. King[3], Mengkun Chen[3], James W. Tunnell[3], Ana Oliveira[4], Pedro Costa[5], Rui Sousa[5], Adriana Mendes[6], Olga Martinho[6], Fatima Baltazar6, Lorena Dieguez[1], Sara Abalde-Cela[1] [1]International Iberian Nanotechnology Laboratory (INL) [2]International Iberian Nanotechnology laboratory (INL) [3]University of Texas at Austin (UTA) [4]Stemmaters Biotecnologia e Medicina Regenerativa SA [5]Stemmaters Biotecnologia e Medicina Regenerativa [6]Life and Health Research Institute (ICVS)
11:40-11:50		**Dual nano-heater and SERS temperature sensor for cancer photothermal therapy** William H. Skinner[1], Renata L. Sala[2], Kamil Sokolowski[2], Jeremy J. Baumberg[2], Oren A. Scherman[2], Benjamin Gardner[1], Pavel Matousek[3], Nicholas Stone[1] [1]University of Exeter [2]University of Cambridge [3]STFC Rutherford Appleton Laboratory
11:55-12:05		**Blood pulse dynamics investigation with non-invasive Raman spectroscopy** Maciej Wróbel[1] [1]Gdansk University of Technology
12:10-13:10		**Lunch**
13:10-14:30		**SESSION 2**
	A1-01	***(I) Chemometrics&machine learning*** Chair: Katarzyna Cieślik-Boczula
13:10-13:25		**Two-trace two-dimensional (2T2D) FTIR correlation spectra applied as input** Bogumiła Kupcewicz[1] [1]Nicolaus Copernicus University, Faculty of Pharmacy

13:30-13:40		**Decoupling of morphological and chemical information in µFTIR spectra using deep learning** Uladzislau Blazhko[1], Eirik Magnussen[1], Johanne Solheim[1], Simona Dzurendova[1], Volha Shapaval[1], Achim Kohler[1] [1]Norwegian University of Life Sciences
13:45-13:55		**Investigation of the bread aging process by handheld NIR spectroscopy in tandem with 2D-COS and MCR-ALS analyses** Marina De Géa Neves[1], Isao Noda[2], Heinz Wilhelm Siesler[1] [1]Department of Physical Chemistry, University Duisburg-Essen [2]Department of Materials Science and Engineering, University of Delaware
14:00-14:10		**Can we follow the metabolism of single leukemic cells using Raman spectroscopy?** Anna M. Nowakowska[1], Aleksandra Borek-Dorosz[1], Patrycja Dawiec[2], Patrycja Leszczenko[2], Adriana Adamczyk[2], Kacper Siakala[1], Justyna Jakubowska[3], Marta Zabczynska[3], Agata Pastorczak[3], Kinga Ostrowska[3], Wojciech Mlynarski[3], Malgorzata Baranska[4], Katarzyna Majzner[1] [1]Jagiellonian University in Krakow, Faculty of Chemistry, Department of Chemical Physics, Krakow, Poland [2]Jagiellonian University in Krakow, Faculty of Chemistry, Department of Chemical Physics, Krakow, Poland; Doctoral School of Exact and Natural Sciences, Jagiellonian University, Krakow, Poland [3]Department of Pediatric, Oncology and Hematology, Medical University of Lodz, Lodz, Poland [4]Jagiellonian University in Krakow, Faculty of Chemistry, Department of Chemical Physics, Krakow, Poland; Jagiellonian University in Krakow, Jagiellonian Centre for Experimental Therapeutics (JCET), Krakow, Poland
	A1-02	***(E) Nonlinear vibrational spectroscopy*** Chair: Xiang Wang
13:10-13:25		**Specific Ion Effects in the Electrical Double Layer Structure at the Silica/Aqueous Interface** Julianne Gibbs[1], Nathaniel Tetteh[1], Shyam Parshotam[1] [1]University of Alberta
13:30-13:45		**Mechanistic Approach to Investigate the Water Evaporation Process at Air/Water Interface using Hofmeister Ions** Bhawna Rana[1], David J. Fairhurst[2], Kailash C. Jena[1] [1]Indian Institute of Technology Ropar [2]Nottingham Trent University
13:50-14:00		**Ultrafast decay of coupled molecule-plasmon nanogap structure** Fiona Bell[1], Lukas Jakob[1], Ishaan Lohia[1], Rakesh Arul[1], Jeremy Baumberg[1] [1]University of Cambridge
14:05-14:15		**How and when does the collapse of a macromolecule in water start? From time-resolved Raman to elastic light scattering viewpoint.** Marcin Pastorczak[1], Michał Nejbauer[1], Naoki Shinyashiki[2], Masanobu Takatsuka[2], Gonzalo Angulo[1], Yuriy Stepanenko[1], Czesław Radzewicz[3] 1Institute of Physical Chemistry Polish Academy of Sciences [2]Department of Physics, School of Science, Tokai University [3]Institute of Experimental Physics, Faculty of Physics, University of Warsaw
14:20-14:30		**Taking Advantage of High Sensitivity Enabled by Stimulated Raman Scattering: Multi-Parameter Analysis of Nanoplastics in Flow** Maximilian Huber[1], Liron Zada[2], Freek Ariese[2], Natalia P. Ivleva[1] [1]Technical University of Munich, Institute of Water Chemistry, Chair of Analytical Chemistry and Water Chemistry, School of Natural Sciences (Dep. Chemistry) [2]Vrije Universiteit Amsterdam, LaserLaB Amsterdam, Department of Physics and Astronomy
	A0-04	***(F) Advances in instrumentation*** Chair: Yuling Wang
13:10-13:20		**Mid-IR Dispersion Spectroscopy – A Powerful Tool for Liquid-Phase Chemical Analysis** Alicja Dabrowska[1], Bernhard Lendl[1] [1]Technische Universität Wien
13:25-13:35		**Raman spectrometer with vertical flow method for organic solvents** Ting-hao Chen[1], Hirotsugu Hiramatsu[1] [1]Department of Applied Chemistry and Institute of Molecular Science, National Yang Ming Chiao Tung University

13:40-13:50		**High-performance miniaturized Raman systems for challenging Raman spectroscopy and microscopy applications** Oleksii Ilchenko[1], Yurii Pilhun[2], Andrii Kutsyk[1], Yaman Goksel[1], Elodie Dumont[1], Thomas Andersen[3], Mikael Lassen[4], Hemanshu Mundhada[5], Christian Jendresen[5], Anja Boisen[1] [1]Technical University of Denmark [2]Lightnovo ApS [3]Odense University Hospital [4]Danish National Metrology Institute [5]Cysbio ApS
13:55-14:05		**A correlated OF2i®-Raman method for micro- and nanoparticle detection and chemical analysis in liquids** Christian Neuper[1], Marko Šimić[2], Christian Hill[3], Werner Grogger4, Harald Fitzek[5] [1]Graz Centre of Electron Microscopy, Steyrergasse 17, Austria / Brave Analytics GmbH, Austria [2]Brave Analytics GmbH, Austria / Gottfried Schatz Research Center, Division of Biophysics, Medical University of Graz, Neue Stiftingtalstraße 2, Graz 8010, Austria / Insitute of Physics, University of Graz, Universitätsplatz 5, Graz 8010, Austria [3]Brave Analytics GmbH, Austria / Gottfried Schatz Research Center, Division of Biophysics, Medical University of Graz, Neue Stiftingtalstraße 2, Graz 8010, Austria [4]Graz Centre of Electron Microscopy, Steyrergasse 17, Austria / Institute of Electron Microscopy and Nanoanalysis, NAWI Graz, Graz University of Technology, Steyrergasse 17, Austria [5]Graz Centre of Electron Microscopy, Steyrergasse 17, Austria
14:10-14:20		**Dielectrophoresis for Raman analysis in liquid: towards a rapid and label-free platform for virus identification** Alessio Sacco[1], Giulia Barzan[1], Slavica Matić[2], Chiara D'Errico[2], Marta Vallino[2], Marina Ciuffo[2], Emanuela Noris[2], Andrea Mario Giovannozzi[1], Chiara Portesi[1], Andrea Mario Rossi[1] [1]National Metrology Research Institute (INRiM) [2]Institute for Sustainable Plant Protection, National Research Council of Italy (CNR)
14:25-14:35		**A Tailored Setup for Multiphase In situ Spectroscopy on Gas-processing Metalloenzymes** Christian Lorent[1], Sagie Katz[1], Vladimir Pelmenschikov[1], Giorgio Caserta[1], Stefan Frielingsdorf[1], Maria Alessandra Martini[2], Konstantin Bikbaev[3], Ingrid Span[3], James A.F. Birrell[4], Oliver Lenz[1], Marius Horch[5], Ingo Zebger[1] [1]Technische Universität Berlin, Insititut für Chemie [2]Max-Planck-Institut für Chemische Energiekonversion [3]Friedrich-Alexander-Universität Erlangen-Nürnberg [4]University of Essex, School of Life Sciences [5]Freie Universität Berlin, Institut für Physik, Biophysik
	A0-03	***(G) Analytical applications*** Chair: Natalia Ivleva
13:10-13:20		**Novel Analytical Approach for Rapid Detection and Characterization of Microplastics in Environmental Samples: Utilizing MIR Spectroscopy's Silent Region for Enhanced Structural Information** Krzysztof B. Bec[1], Justyna Grabska[1], Jovan Badzoka[1], Christian W. Huck[1] [1]University of Innsbruck
13:25-13:35		**Quantification of microplastics in environmental samples through a combination of optical and FTIR- and Raman microspectroscopy enhanced by Machine Learning evaluation** Dieter Fischer[1], Kristina Enders[1], Robin Lenz[1], Franziska Fischer[2], Elisavet Kanaki[1], Julia Muche[1], Benedikt Hufnagl[3] [1]Leibniz-Institut für Polymerforschung Dresden [2]Advanced Mask Technology Center GmbH Dresden [3]Purency GmbH Wien
13:40-13:50		**Comparison of Raman- and fluorescence techniques for detection and identification of micro-plastics in environmental samples** Merel Konings[1], Liron Zada[1], Robert Schmidt[1], Freek Ariese[1] [1]Vrije Universiteit Amsterdam
13:55-14:05		**Applications of optical photothermal infrared spectroscopy (O-PTIR) in plastic pollution research: from detecting microplastics to monitoring the production of microbial bioplastic** Cassio Lima[1], Howbeer Muhamadali[1], Royston Goodacre[1] [1]University of Liverpool

14:10-14:20		**Nanoscale chemical characterization is crucial for polymer recycling** Georg Ramer[1], V. D. Dos Santos A. Catarina[1], Lena Neubauer[2], Bernhard Lendl[2] [1]TU Wien / Institute for chemical Technologies and Analytics [2]TU Wien / Institute for chemical Technologie and Analytics
14:25-14:35		**In-line near-infrared spectroscopic monitoring for injection molding of biodegradable polymer blends** Itsuki Yoshikawa[1], Yuta Hikima[1], Masahiro Ohshima[1] [1]Kyoto University
	A0-01	***(H) Biodiagnostic spectroscopy*** Chair: Peter Gardner
13:10-13:20		**Rapid identification of bacteria isolated directly from patient urine and diagnosis of their antibiotic susceptibility using infrared spectroscopy-based machine learning** George Abu-Aqil[1], Manal Suleiman[1], Uraib Sharaha[1], Lior Nesher[2], Itshak Lapidot[3], Ahmad Salman[4], Mahmoud Huleihel[1] [1]Ben-Gurion University of the Negev [2]Soroka University Medical Center [3]Afeka Tel-Aviv Academic College of Engineering [4]Shamoon College of Engineering
13:25-13:35		**Supplementation of vitamin C and E – an effect on human gastrointestinal tract tissues and cells: Raman spectroscopy and imaging** Karolina Beton-Mysur[1], Beata Brożek-Płuska[1] [1]Lodz University of Technology, Faculty of Chemistry, Institute of Applied Radiation Chemistry, Laboratory of Laser Molecular Spectroscopy
13:40-13:50		**Molecular Characterisation of T-cell acute lymphoblastic leukemia using Raman spectroscopy** Patrycja Dawiec[1], Patrycja Leszczenko[1], Anna Nowakowska[2], Karolina Czuja[2], Justyna Jakubowska[3], Marta Zabczyńska[3], Agata Pastorczak[3], Kinga Ostrowska[3], Wojciech Mlynarski[3], Malgorzata Baranska[4], Katarzyna Majzner[2] [1]Jagiellonian University in Krakow, Faculty of Chemistry, Department of Chemical Physics; Doctoral School of Exact and Natural Sciences [2]Jagiellonian University in Krakow, Faculty of Chemistry, Department of Chemical Physics [3]Department of Pediatrics, Oncology and Hematology, Medical University of Lodz [4]Jagiellonian University in Krakow, Faculty of Chemistry, Department of Chemical Physics; Jagiellonian University in Krakow, Jagiellonian Centre for Experimental Therapeutics
13:55-14:05		**Raman-based assessment of the endothelial response to antiretroviral drugs: in vitro studies on NNRTI-treated human endothelial cells** Jagoda Orleanska[1], Wiktoria Wiecek[2], Malgorzata Baranska[3], Katarzyna Majzner[2] [1]1 Jagiellonian University, Faculty of Chemistry, Department of Chemical Physics, Krakow, Poland; 2 Doctoral School of Exact and Natural Sciences, Jagiellonian University in Krakow, Krakow, Poland [2]1 Jagiellonian University, Faculty of Chemistry, Department of Chemical Physics, Krakow, Poland [3]1 Jagiellonian University, Faculty of Chemistry, Department of Chemical Physics, Krakow, Poland; 3 Jagiellonian University in Krakow, Jagiellonian Centre for Experimental Therapeutics (JCET), Krakow, Poland
14:10-14:20		**Bladder Cancer detection by Fourier Transform Infrared Spectroscopy (FTIR) using urine samples.** Imane Oudahmane[1], Fayek Taha[2], Elie Sarkees[1], Jade Vanmansart[1], Vincent Vuiblet[3], Stéphane Larre[2], Olivier Piot[1] [1]BioSpecT (Translational BioSpectroscopy) EA 7506. Université de Reims Champagne-Ardenne. [2]Department of Urology, University Hospital of Reims. [3]Department of Biopathology, University Hospital of Reims.
14:25-14:35		**Exploring the potential for Deep Raman Spectroscopy for non-invasive sex determination of chicken eggs** Lennard Van den Tweel[1], Freek Ariese[2], Carla Van der Pol[3], Henry Van den Brand[1] [1]Adaptation Physiology Group, Wageningen University & Research [2]LaserLaB, Department of Physics and Astronomy, Vrije Universiteit Amsterdam [3]Research Department, HatchTech B.V.
14:30-15:00		**Coffee Break**
15:00-16:15		**SESSION 3**
	A1-01	***(I) Chemometrics&machine learning*** Chair: Stefania Dana Iancu

15:00-15:10		**Advancing cancer stem cell detection through line illumination Raman microscope and hydrogel substrate.** Jean-Emmanuel Clément[1], Zannatul Ferdous[1], Thomas Bocklitz[2], Katsumasa Fujita[3], Jian Ping Gong[1], Shinya Tanaka[1], Tamiki Komatsuzaki[1] [1]Hokkaido University-ICReDD [2]University of Bayreuth [3]Osaka University
15:15-15:25		**Discrimination between chemoresistant and chemosensitive ovarian cancer cells with confocal Raman microscopy** Elina Harju[1], Teemu Tomberg[1], Sara Fraser-Miller[2], Jukka Saarinen[1], Kathleen J. Sircombe[3], Sarah Hook[3], Keith C. Gordon[2], Clare J. Strachan[1] [1]Division of Pharmaceutical Chemistry and Technology, Faculty of Pharmacy, University of Helsinki [2]The Dodd-Walls Centre for Photonic and Quantum Technologies – Te Whai Ao and Department of Chemistry, University of Otago [3]School of Pharmacy, University of Otago
15:30-15:40		**Can we diagnose the KMT2A leukemia subtype with Raman microscopy?** Patrycja Leszczenko[1], Anna M. Nowakowska[1], Justyna Jakubowska[2], Agata Pastorczak[2], Marta Zabczynska[2], Wojciech Mlynarski[2], Malgorzata Baranska[1], Kinga Ostrowska[2], Katarzyna Majzner[1] [1]Faculty of Chemistry, Jagiellonian University [2]Department of Pediatric, Oncology and Hematology, Medical University of Lodz
15:45-15:55		**Pretreatment routines in analysis of Raman spectra recorded in different excitation wavelength and its effect on classification models** Sara Mostafapour[1], Thomas Dörfer[2], Ralf Henke[2], Petra Rösch[2], Jürgen Popp[1], Thomas Bocklitz[3] [1]1.Leibniz Institute of Photonic Technology, Jena, Germany/2. Institute of Physical Chemistry and Abbe Centre of Photonics, Friedrich Schiller University of Jena, Jena, Germany [2]Institute of Physical Chemistry and Abbe Centre of Photonics, Friedrich Schiller University of Jena, Jena, Germany [3]1.Leibniz Institute of Photonic Technology, Jena, Germany/2. Institute of Physical Chemistry and Abbe Centre of Photonics, Friedrich Schiller University of Jena, Jena, Germany/3. Institute of Computer Science, Faculty of Mathematics, Physics & Computer Sc
16:00-16:10		**Infrared molecular fingerprinting for multi-phenotyping of human health and disease** Kepesidis V. Kosmas[1], Marinus Huber[2], Liudmila Voronina[1], Tarek Eissa[1], Frank Fleischmann[1], Cristina Leonardo[1], Jacqueline Hermann[1], Ina Koch[3], Thomas Kolben[4], Gerald Schulz[5], Friedrich Jokisch[5], Juergen Behr[6], Nadia Harbeck[4], Maximilian Reiser[7], Christian Stief[5], Ferenc Krausz[1], Mihaela Zigman[1] [1]Ludwig Maximilian University of Munich (LMU) [2]Max Planck Institute of Quantum Optics (MPQ) [3]Asklepios Biobank for Lung Diseases, Department of Thoracic Surgery, Member of the German Center for Lung Research, DZL, Asklepios Fachkliniken München-Gauting [4]University Hospital of the Ludwig Maximilians University Munich (LMU), Department of Obstetrics and Gynecology, Breast Center and Comprehensive Cancer Center (CCLMU) [5]University Hospital of the Ludwig Maximilians University Munich (LMU), Department of Urology [6]University Hospital of the Ludwig Maximilians University Munich (LMU), Department of Internal Medicine V [7]University Hospital of the Ludwig Maximilians University Munich (LMU), Department of Clinical Radiology
	A1-02	***(E) Nonlinear vibrational spectroscopy*** Chair: Marcin Pastorczak
15:00-15:10		**Raman and Stimulated Raman Scattering characterization of carotenoids and amyloid beta deposits in Alzheimer's Disease brain samples** Freek Ariese[1], Benjamin Lochocki[2], Liron Zada[1], Loes Ettema[1], Can Keskin[1], Jinke Van der Sluis[1], Robert W. Schmidt[1] [1]LaserLaB, Vrije Universiteit [2]ARCNL

15:15-15:25		**Glucose and lipid metabolism in endothelium inflammation studied by Raman microscopy** Aleksandra Borek-Dorosz[1], Anna Pieczara[2], Jagoda Orleańska[3], Krzysztof Brzozowski[1], William Tipping[4], Duncan Graham[4], Malgorzata Baranska[5], Katarzyna Majzner[1] [1]1 Jagiellonian University in Kraków, Faculty of Chemistry, Department of Chemical Physics, 2 Gronostajowa Str., Krakow, Poland [2]2 Jagiellonian University in Kraków, Jagiellonian Centre for Experimental Therapeutics (JCET), 14 Bobrzynskiego Str., Krakow, Poland 3 Jagiellonian University in Kraków, Doctoral School of Exact and Natural Sciences, 11 Lojasiewicza St., Krakow, Poland [3]1 Jagiellonian University in Kraków, Faculty of Chemistry, Department of Chemical Physics, 2 Gronostajowa Str., Krakow, Poland 3 Jagiellonian University in Kraków, Doctoral School of Exact and Natural Sciences, 11 Lojasiewicza St., Krakow, Poland [4]4 Centre for Molecular Nanometrology, WestCHEM, Department of Pure and Applied Chemistry, Technology and Innovation Centre, University of Strathclyde, Glasgow G1 1RD, United Kingdom [5]1 Jagiellonian University in Kraków, Faculty of Chemistry, Department of Chemical Physics, 2 Gronostajowa Str., Krakow, Poland 2 Jagiellonian University in Kraków, Jagiellonian Centre for Experimental Therapeutics (JCET), 14 Bobrzynskiego Str., Krakow, Poland
15:30-15:40		**Stimulated Raman scattering imaging – 3D spatial generation** Ronja Eriksson[1], Per Gren[1], Mikael Sjödahl[1], Kerstin Ramser[1] [1]Department of Engineering Sciences and Mathematics, Luleå University of Technology
15:45-15:55		**Modified glucose as a probe to track the metabolism in single endothelial cells – observation of the 1602 cm-1 band called "Raman spectroscopic signature of life"** Anna Pieczara[1], Aleksandra Borek-Dorosz[1], Szymon Buda[1], William Tipping[2], Duncan Graham[2], Robert Pawlowski[3], Jacek Mlynarski[3], Malgorzata Baranska[1] [1]Jagiellonian University [2]University of Strathclyde [3]Polish Academy of Sciences
16:00-16:10		**Stimulated Raman scattering (SRS) microscopy to investigate pharmaceutical co-crystal formation** Oona Auvinen[1], Alba Arbiol[1], Tom Konings[1], Teemu Tomberg[1], Leena Peltonen[1], Clare Strachan[1], Jukka Saarinen[1] [1]Division of Pharmaceutical Chemistry and Technology, Faculty of Pharmacy, University of Helsinki
	A0-04	***(A) Advanced characterization of materials*** Chair: Justyna Grabska
15:00-15:15		**Inside block copolymer micelles – An AFM-TERS study on the interfacial influences on the core crosslinking efficiency** Christiane Höppener[1], Xinyue Wang[2], Johanna Elter[3], Felix Schacher[3], Volker Deckert[1] [1]Leibniz Institute of Photonic Technologies (IPHT) [2]Institute of Physical Chemistry, Friedrich Schiller University [3]Institute of Organic Chemistry and Macromolecular Chemistry, Friedrich Schiller University
15:20-15:35		**Towards the compactness and permeability of the polymer brushes studied by surface-enhanced Raman spectroscopy** Marek Procházka[1], Monika Spasovová[2], Markéta Vrabcová[2], Josef Štěpánek[1], Ondřej Kylián[3], Hana Vaisocherová-Lísalová[4] [1]Institute of Physics, Faculty of Mathematics and Physics, Charles University [2]Department of Optical and Biophysical Systems, Institute of Physics of the Czech Academy of Sciences; Institute of Physics, Faculty of Mathematics and Physics, Charles University [3]Department of Macromolecular Physics, Faculty of Mathematics and Physics, Charles University [4]Department of Optical and Biophysical Systems, Institute of Physics of the Czech Academy of Sciences
15:40-15:50		**Characterisation and evaluation of molecularly imprinted polymers using surface enhanced infrared absorption (SEIRA) spectroscopy.** Armel F. T. Waffo[1], Sagie Katz[1], Giorgio Caserta[1], Aysu Yarman[2], Bettina Neumann[3], Ulla Wollenberger[3], Frieder W. Scheller[3] [1]Technische Universität Berlin [2]Turkish-German University [3]University of Potsdam

15:55-16:05		**Enhancement of the E12g and A1g Raman modes and Layer Identification of 2H-WS2 Nanosheets With Metal Coatings** Bharathi Rajeswaran[1], Rajashree Konar[1], Gilbert Daniel Nessim[2], Yaakov Raphael Tischler[1] [1]Bar-Ilan University, Israel [2]Bar-Ilan University, Ramat Gan, Israel
	A0-03	***(G) Analytical applications*** Chair: Maria-Paula Marques
15:00-15:15		**Insights into forensic analysis of peripheral blood stains on natural and synthetic fabrics using ATR-FTIR spectroscopy** Entesar Al-Hetlani[1], Zainab Husain[1], Mohamed Amin[1] [1]Kuwait University
15:20-15:35		**Revealing the Secrets of Graeco-Roman Egyptian Mummies Using Vibrational Spectroscopic Techniques** Bayden Wood[1], Callum Gassner[1], Magdalena Giergiel[1], Ankit Dodla[1], Janet Davey[2] [1]Monash University [2]Victorian Institute of Forensic Medicine
15:40-15:50		**Fingermark analysis utilizing ATR-FTIR spectroscopy for forensic discrimination of smoker and nonsmoker** Mohamed O. Amin[1], Entesar Al-Hetlani[1], Igor K. Lednev Lednev[2] [1]Kuwait University [2]University at Albany
15:55-16:05		**Deep UV Raman spectroscopy for post-mortem interval determination** Anna Wójtowicz[1], Luis Perez Almodovar[2], Igor K. Lednev[2], Renata Wietecha-Posłuszny[1] [1]Laboratory for Forensic Chemistry, Department of Analytical Chemistry, Faculty of Chemistry, Jagiellonian University [2]Department of Chemistry, University at Albany, SUNY
	A0-01	***(H) Biodiagnostic spectroscopy*** Chair: Hugh Byrne
15:00-15:10		**Raman-based evaluation of in vitro myeloid precursor differentiation toward macrophages** Adriana Adamczyk[1], Anna Nowakowska[1], Justyna Jakubowska[2], Katarzyna Majzner[1], Malgorzata Baranska[1] [1]Jagiellonian University in Krakow, Faculty of Chemistry, Department of Chemical Physics, Kraków, Poland [2]Department of Pediatrics, Oncology and Hematology, Medical University of Lodz, Łódz, Poland
15:15-15:25		**Brillouin and Raman micro-spectroscopy to characterise human bone and cartilage: from healthy phenotype to biomedical applications in osteoarthritis and bone infections.** Martina Alunni Cardinali[1], Sara Stefani[1], Marco Govoni[2], Dante Dallari[2], Leonardo Vivarelli[2], Matilde Tschon[3], Silvia Brogini[3], Alessandra Maso[4], Elisa Storni[4], Francesca Valenti[5], Melania Maglio[3], Maurizio Mattarelli[6], Alessandra Anna Passeri[6], Silvia Caponi[7], Assunta Morresi[1], Paola Sassi[1], Daniele Fioretto[6] [1]Dep. Chemistry, Biology and Biotechnology, University of Perugia [2]Reconstructive Orthopaedic Surgery and Innovative Techniques – Musculoskeletal Tissue Bank, IRCCS Istituto Ortopedico Rizzoli [3]Surgical Sciences and Technologies, IRCCS Istituto Ortopedico Rizzoli [4]Laboratory of Microbiology and GMP Quality Control, IRCCS Istituto Ortopedico Rizzoli [5]Dep. of Pharmacy and Biotechnology, University of Bologna [6]Dep. Physics and Geology, University of Perugia [7]CNR- Dep. Physics and Geology
15:30-15:40		**Fourier Transform Infrared Microspectroscopy identifies single cancer cells in blood. A feasibility study towards liquid biopsy.** Lewis M. Dowling[1], Paul Roach[2], Eirik A. Magnussen[3], Achim Kohler[3], Srinivas Pillai[4], Daniel G. Van Pittius[4], Ibraheem Yousef[5], Josep Sulé-Suso[1] [1]Keele University [2]Loughborough University [3]Norwegian University of Life Sciences [4]University Hospitals of North Midlands [5]ALBA Synchrotron Light Source

15:45-15:55		**Raman spectroscopy in the biochemical characterisation of THP-1 leukemic cells modified to overexpress mutated FLT3 receptor.** Sylwia Orzechowska[1], Paulina Laskowska[2], Aleksandra Borek-Dorosz[1], Anna Maria Nowakowska[1], Wiktoria Korona[1], Marcin Szydłowski[2], M. Zasowska[2], Piotr Juszczyński[2], Małgorzata Barańska[3], Piotr Mrówka[4], Katarzyna Majzner[1] [1]Jagiellonian University, Faculty of Chemistry [2]Department of Experimental Hematology, Institute of Hematology and Transfusion Medicine [3]Jagiellonian University, Faculty of Chemistry; Jagiellonian Centre for Experimental Therapeutics (JCET), Jagiellonian University [4]Department of Experimental Hematology, Institute of Hematology and Transfusion Medicine; Department of Biophysics, Physiology and Pathophysiology, Medical University of Warsaw
16:00-16:10		**Identification of Chemical Modifications of Myocardium in Heart-Failure with Preserved Ejection Fraction** Leonardo Pioppi[1], Reza Parvan[2], Alan Samrend[2], Gustavo Jose Justo Da Silva[2], Marco Paolantoni[1], Alessandro Cataliotti[2], Paola Sassi[1] [1]Department of Chemistry, Biology and Biotechnology, University of Perugia [2]Institute for Experimental Medical Research, Oslo University Hospital and University of Oslo
16:30-18:45		**POSTER SESSION 3: Topics G, H, I**
		Chairs: Sara Miller, Christian Johannessen
16:30-17:30	A0-01	Flash Presentations
17:30-18:45		Poster Session

Thursday		
9:00-10:15	**A0-01**	**Plenary Session**
		Chair: Pavel Matousek
9:00-9:30		Raman Imaging of Plant Cells: probing distribution and orientation of molecules Notburga Gierlinger[1] [1]University of Natural Resources and Life Sciences Vienna (BOKU)
		Chair: Petra Hellwig
9:40-10:10		**Theory is dead, long live theory: Hypothesis-centric machine learning in vibrational spectroscopy** Axel Mosig[1] [1]Ruhr University Bochum, Center for Protein Diagnostics
10:15-10:45		**Coffee Break**
10:45-12:10		**SESSION 1**
	A1-01	***(I) Chemometrics&machine learning*** Chair: Alicja Dąbrowska
10:45-10:55		**Spatially offset low frequency Raman spectroscopy for discriminating microcalcifications immersed and under varying depths of paraffin wax** Mitchell Chalmers[1], Sara Miller[1], Teemu Tomberg[2], Keith Gordon[1] [1]Te Whai Ao – The Dodd-Walls Centre for Photonic and Quantum Technologies and Department of Chemistry, University of Otago [2]Division of Pharmaceutical Chemistry and Technology, Faculty of Pharmacy, University of Helsinki
11:00-11:10		**The data exploring expedition. A practical outline to processing and investigation of experimental spectra with the selected methods of chemometric data modeling** Andrzej J. Kałka[1], Andrzej M. Turek[1] [1]Jagiellonian University in Cracow, Faculty of Chemistry
11:15-11:25		**RamApp: a modern web-based toolbox for the processing and analysis of hyperspectral imaging data** Elia Broggio[1], Andrea Masella[1], Giulia De Poli[1], Manuela Bazzarelli[1], Dario Polli[2], Matteo Bregonzio[1], Renzo Vanna[3] [1]Datrix S.p.A. [2]Department of Physics, Politecnico di Milano / Istituto di Fotonica e Nanotecnologie (IFN), Consiglio Nazionale delle Ricerche (CNR) [3]Istituto di Fotonica e Nanotecnologie (IFN), Consiglio Nazionale delle Ricerche (CNR)
11:30-11:40		**Tensor decomposition assisted super-resolution in polarized Raman microscopy** Andrii Kutsyk[1], Oleksii Ilchenko[1], Yurii Pilhun[2], Jens Wenzel Andreasen[1] [1]Technical University of Denmark [2]Lightnovo ApS
11:45-11:55		**Extensive Evaluation of Machine Learning Models and Data Preprocessings for Raman Modeling in Bioprocessing** Michaela Poth[1], Gordon Magill[2], Alois Filgertshofer[1], Oliver Popp[1], Tobias Großkopf[1] [1]Therapeutic Modalities, Roche Innovation Center Munich, Bioprocess Research, Roche Pharma Research and Early Development [2]Cell Culture Development and Bioprocess, Genentech Inc.
12:00-12:10		**Pre-Processing and Unsupervised Unmixing of Hyperspectral Raman Datasets with RamanLIGHT** Robert W. Schmidt[1], Sander Woutersen[2], Freek Ariese[1] [1]Vrije Universiteit Amsterdam [2]University of Amsterdam
	A1-02	***(E) Nonlinear vibrational spectroscopy*** Chair: Zsuzsanna Heiner
10:45-11:00		**Nonlinear Vibrational Spectroscopy as an Orientation-Independent Probe of Molecular Environments at Interfaces** Dennis Hore[1], Aruna Kumarasiri[1], Peter Yang[1] [1]University of Victoria
11:05-11:20		**Molecular-Level Elucidation of Buried Solid/Liquid Interfaces by the Use of Heterodyne-detected Vibrational Sum Frequency Generation** Satoshi Nihonyanagi[1] [1]Molecular Spectroscopy Lab., RIKEN

11:25-11:35		**Investigating Viscoelastic Induced Nature at Air-Aqueous Interface by Nonlinear Laser Vibrational Spectroscopy** Sarabjeet Kaur[1], Kailash Chandra Jena[1] [1]Indian Institute of Technology Ropar
11:40-11:50		**Unraveling the sign of excited-state molecular displacements via broadband impulsive Raman spectroscopy** Giovanni Batignani[1], Emanuele Mai[1], Giuseppe Fumero[2], Shaul Mukamel[3], Tullio Scopigno[4] [1]Physics Department, Sapienza University of Rome, Rome, Italy; Italian Institute of Technology, Center for Life Nano Science @Sapienza, Rome, Italy [2]Physics Department, Sapienza University of Rome, Rome, Italy [3]Department of Chemistry, University of California, Irvine, CA, USA [4]Physics Department, Sapienza University of Rome, Rome, Italy; Italian Institute of Technology, Center for Life Nano Science @Sapienza, Rome, Italy; Italian Institute of Technology, Graphene Labs, Genoa, Italy
11:55-12:05		**Charge Transfer Across Hydrophobic Interfaces** Saranya Pullanchery[1], Sergey Kulik[1], Benjamin Rehl[1], Ali Hassanali[2], Sylvie Roke[1] [1]Laboratory for Fundamental BioPhotonics, Institute of Bioengineering (IBI), School of Engineering (STI), École Polytechnique Fédérale de Lausanne (EPFL) [2]The Abdus Salam International Centre for Theoretical Physics
	A0-04	***(A) Advanced characterization of materials*** Chair: Valentina Notarstefano
10:45-10:55		**Ibuprofen/chitosan matrices as a promising base for intestinal soft capsules** Barbara Gieroba[1], Maryna Khalavka[2], Olena Mozgova[3], Paulina Kazimierczak[4], Grzegorz Kalisz[1], Izabela S. Pięta[5], Liudmyla Nosach[6], Vladyslav Vivcharenko[4], Agata Przekora[4], Anna Sroka-Bartnicka[1] [1]Independent Unit of Spectroscopy and Chemical Imaging, Faculty of Biomedical Sciences, Medical University of Lublin, Chodzki 4a, 20-093 Lublin, Poland [2]Independent Unit of Spectroscopy and Chemical Imaging, Faculty of Biomedical Sciences, Medical University of Lublin, Chodzki 4a, 20-093 Lublin, Poland; Department of Industrial Technology of Drugs, National University of Pharmacy, Pushkins'ka 63 St., 6100 [3]Independent Unit of Spectroscopy and Chemical Imaging, Faculty of Biomedical Sciences, Medical University of Lublin, Chodzki 4a, 20-093 Lublin, Poland; National University of Pharmacy, Department of Inorganic and Physical Chemistry, Valentynivska 4 St., 6 [4]Independent Unit of Tissue Engineering and Regenerative Medicine, Faculty of Biomedical Sciences, Medical University of Lublin, Chodzki 1, 20-093 Lublin, Poland [5]Institute of Physical Chemistry Polish Academy of Sciences, Kasprzaka 44/52, 01-224 Warsaw, Poland [6]Independent Unit of Tissue Engineering and Regenerative Medicine, Faculty of Biomedical Sciences, Medical University of Lublin, Chodzki 1, 20-093 Lublin, Poland; Department of Amorphous and Structurally Ordered Oxides, Chuiko Institute of Surface Chemistr
11:00-11:10		**Low frequency Raman spectroscopy for characterization of amorphous and crystalline variably substituted hydroxyapatites** Joshua Kirkham[1], Tim Kortner[2], Kārlis Bērziņš[1], Cushla McGoverin[3], Keith Gordon[1], Sara Miller[1] [1]Te Whai Ao – The Dodd-Walls Centre for Photonic and Quantum Technologies and Department of Chemistry, University of Otago [2]Department of Chemistry, Syracuse University, Center for Science and Technology [3]Te Whai Ao – The Dodd-Walls Centre for Photonic and Quantum Technologies, and Department of Physics, University of Auckland
11:15-11:25		**Exploring the glycosaminoglycan structure: does it fold and how?** Gergo Peter Szekeres[1], Jan Horlebein[2], Jerome Riedel[1], Gert Von Helden[2], Mark Mero[3], Kevin Pagel[1], Zsuzsanna Heiner[4] [1]Freie Universität Berlin, Fritz-Haber-Institut der Max-Planck-Gesellschaft [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft [3]Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy [4]School of Analytical Sciences Adlershof, Humboldt-Universität zu Berlin
11:30-11:40		**Phosphine Halogen-Bonded Complexes: Investigated Using Matrix Isolation IR Spectroscopy** Elliot Tay[1], Corentin Grassin[1], Clemens Müller[1], Christian Merten[1] [1]Organische Chemie II, Fakultät für Chemie und Biochemie

11:45-11:55		**Raman spectroscopy for investigation of interaction within polymer based magnetic multicomponent scaffolds** Anna Kołodziej[1], Małgorzata Świętek[2], Anna Hlukhaniuk[2], Daniel Horák[2], Aleksandra Wesełucha-Birczyńska[1] [1]Faculty of Chemistry, Jagiellonian University [2]Institute of Macromolecular Chemistry, Czech Academy of Sciences
12:00-12:10		**Which method will distinguish nanofibrous carbon materials?** Aleksandra Wesełucha-Birczyńska[1], Maria Pajda[2], Elżbieta Długoń[3], Krzysztof Morajka[1], Marek Michalec[1], Marta Błażewicz[4] [1]Faculty of Chemistry, Jagiellonian University [2]Technolutions [3]AGH – University of Science and Technology, Faculty of Materials Science and Ceramics, [4]AGH – University of Science and Technology, Faculty of Materials Science and Ceramics
	A0-03	***(D) Spectroscopy of surface&interfaces*** Chair: Inez Weidinger
10:45-11:00		**Surface-enhanced resonance Raman spectro-electrochemistry as a tool to study redox-related structural changes in (bio)chemistry in-situ** Michelle Mahler1, Patrycja Kielb[1] [1]University of Bonn
11:05-11:20		**Tip-enhanced Raman spectroscopy for nanoscale studying of catalytic. systems** Bin Ren[1], Xiang Wang[1], Tengxiang Huang[1], Huishu Feng[1] [1]Xiamen University
11:25-11:35		**Mechanistic insights of conjugated acetylenic polymers for the photoelectrochemical nitrogen reduction reaction to ammonia** Mino Borrelli[1], Agnieszka Kuc[2], Xinliang Feng[1], Inez Weidinger[1] [1]TUD [2]Helmholtz-Zentrum Dresden-Rossendorf
11:40-11:50		**Revealing the Size Effect of Pd/Au Bimetallic Catalysts at Nanoscale with Tip-enhanced Raman Spectroscopy** Xiang Wang[1], Hui-shu Feng[1], Hai-sheng Su[1], Ya-qiong Su[2], Bin Ren[1] [1]Xiamen University [2]Xi'an Jiaotong University
11:55-12:05		**The study of correlated Stokes-and-anti-Stokes in normal Raman and in Surface-Enhanced Raman Scattering (SERS)** Filomeno Aguiar Junior[1], Sahar Milani[1], Sanker Timsina[2], Stanislav Konorov[1], Michele L. de Souza[1], Rogério De Sousa[3], Alexandre Brolo[1] [1]Department of Chemistry, University of Victoria-BC [2]Department of Physics , University of Victoria-BC [3]Department of Physics, University of Victoria-BC
	A0-01	***(H) Biodiagnostic spectroscopy*** Chair: Michael Heise
10:45-11:00		**Raman imaging and AFM studies of human colon tissues and cells – cholesterol impact on CRC development** Beata Brozek-Pluska[1], Karolina Beton-Mysur[1] [1]Lodz University of Technology, Faculty of Chemistry, Laboratory of Laser Molecular Spectroscopy
11:05-11:20		**Raman Spectroscopy for Pre-Disease Analysis** Pradjna Paramitha[1], Keita Iwasaki[1], Kosuke Hashimoto[1], Bibin Andriana[1], Hidetoshi Sato[1] [1]Department of Biological and Environmental Sciences, Kwansei Gakuin University
11:25-11:35		**Application of Raman spectroscopy to examine tattoo pigments in tissues** Katarzyna Karpienko[1], Aneta Szczerkowska-Dobosz[2], Patrycja Rogowska[2], Iwona Kaczmarzyk[1], Maciej S. Wróbel[1] [1]Department of Metrology and Optoelectronics, Faculty of Electronics, Telecommunication and Informatics, Gdansk University of Technology [2]Department of a Department of Dermatology, Venereology and Allergology, Faculty of Medicine, Medical Univeristy of GdańskMetrology and Optoelectronics, Faculty of Electronics, Telecommunication and Informatics, Gdansk University of Technology

11:40-11:50		**Raman analysis of breast microcalcifications, correlation with pathology** Carlo Morasso[1], Renzo Vanna[2], Francesca Piccotti[1], Marta Truffi[1], Sara Albasini[1], Thomas Huthwelker[3], Laura Villani[1], Oliver Bunk[3], Cinzia Giannini[4], Fabio Corsi[5] [1]Istituti Clinici Scientifici Maugeri IRCCS [2]Institute for Photonics and Nanotechnologies, National Research Council (IFN-CNR) [3]Paul Scherrer Institut [4]Institute of Crystallography, National Research Council [5]Department of Biomedical and Clinical Sciences, University of Milan
11:55-12:05		**Pre-clinical characterization of Osteopetrosis in Mice Models by Raman microspectroscopy** Marco Ventura[1], Alejandro De La Cadena[1], Morteza Behrouzitabar[2], Maria Lucia Schiavone[3], Federico Vernuccio[2], Giulio Cerullo[2], Cristina Sobacchi[3], Dario Polli[2], Renzo Vanna[1] [1]CNR-IFN [2]Politecnico di Milano [3]IRCCS Humanitas Researc Hospital
12:10-13:10		Lunch
13:10-14:30		SESSION 2
	A1-01	(I) Chemometrics&machine learning Chair: Valeria Tafintseva
13:10-13:20		**Long short-term memory and Transformer in Classification and Correction of ATR distorted spectrum** Rui Cheng[1], Johannes Kiefer[1] [1]University of Bremen
13:25-13:35		**Classifying Cheddar cheese based on maturity level and manufacturer using vibrational spectroscopy and chemometrics.** Gerson R. Dewantier[1], Peter J. Torley[1], Ewan W. Blanch[1] [1]RMIT University
13:40-13:50		**Characterization of root tissue development associated with lodging tendency in tef using Raman micro-spectroscopyscopy** Sabrina Diehn[1], Noa Kirby[1], Shiran Ben-Zeev[1], Yehoshua Saranga[1], Rivka Elbaum[1] [1]The Robert H Smith Faculty of Agriculture, Food and Environment, Hebrew University of Jerusalem
13:55-14:05		**Plasmonic surface enhanced infrared spectroscopy aided with artificial intelligence for structural protein biomarker based neurodegenerative disease detection** Deepthy Kavungal[1], Pedro Magalhães[2], Senthil Kumar[2], Rajasekhar Kolla[2], Hilal Lashuel[2], Hatice Altug[1] [1]Institute of Bioengineering, EPFL [2]Brain Mind Institute, EPFL
14:10-14:20		**The use of NIR spectroscopy for the analysis of Fumonisin B1 (FB1)** Anja Laubscher[1], Paul J. Williams[1], Lindy J. Rose[1] [1]Stellenbosch University
14:25-14:35		**A multivariate surface-enhanced infrared absorption (SEIRA) method based on quantum dots and universal attenuated total reflectance (UATR) accessory for atrazine determination** Felipe Trindade[1], Izabel Souza Sobrinha[1], Giovannia Pereira[1], Claudete Pereira[1] [1]Universidade Federal de Pernambuco
	A1-02	***(J) Computational approaches*** Chair: James Cheeseman
13:10-13:25		**Raman Optical Activity: Simulations Outside and In Resonance** Petr Bour[1] [1]Institute of Organic Chemistry and Biochemistry
13:30-13:45		**CHIROPTICAL SPECTRA: WHEN CALCULATIONS MEET THE EXPERIMENT** Joanna E. Rode[1] [1]Institute of Nuclear Chemistry and Technology, Dorodna 16
13:50-14:00		**A study of synchrotron-based UV-resonance Raman spectra of N-acetylamino saccharides – In combination with their ATR-far ultraviolet spectroscopy study** Kousuke Hashimoto[1], Fatima Matroodi[2], Mariagrazia Tortra[2], Barbara Rossi[2], Yusuke Morisawa[3], Yukihiro Ozaki[1], Hidetoshi Sato[1] [1]School of Biological and Environmental Sciences, Kwansei Gakuin University [2]Elettra – Sincrotrone Trieste [3]School of Science and Engineering, Kindai University

14:05-14:15		**Vibrational Circular Dichroism of Chiral Crystals: The Interplay of Symmetry and Chirality** Sascha Jähnigen[1], Anne Zehnacker[2], Rodolphe Vuilleumier[1] [1]Ecole Normale Supérieure [2]Institut des Sciences Moléculaires d'Orsay, Université Paris-Saclay
14:20-14:30		**Infrared spectrum, Barrier heights and Density Functional Theory calculations of N-(n-Butyl)-N'-[(p-Chloro phenoxy) acetyl] Urea** J Sunil[1], Kanugula Srishailam[1], B Venkatram Reddy[2], G Ramana Rao[2] [1]SR University [2]Kakatiya University
14:35-14:45		**Quantitative evaluation of IR and corresponding VCD spectra** Thomas Mayerhöfer[1], Ankit Singh[1], Jer-shing Huang[1], Christoph Krafft[1], Juergen Popp[1] [1]Leibniz Institute of Photonic Technology
	A0-04	***(A) Advanced characterization of materials*** Chair: Ana Batista de Carvalho
13:10-13:20		**Raman Confocal Imaging for materials at high temperatures** Maciej Bik[1], Piotr Jeleń[1], Maciej Sitarz[1] [1]AGH University of Science and Technology, Faculty of Materials Science and Ceramics
13:25-13:35		**Automated Quantitative Analysis of (Microplastic) Particles and Fibers down to 1 µm by Raman Microspectroscopy** Oliver Jacob[1], Alejandro Ramírez-Piñero[1], Natalia Ivleva[1] [1]Chair of Analytical Chemistry and Water Chemistry, Technical University of Munich
13:40-13:50		**Investigating Degradation of Poly(vinyl chloride) by Spectroscopic Methods** Marwa Saad[1], Krzysztof Kruczała[1], Marek Bucki[1], Karol Górecki[1], Sonia Bujok[2], Łukasz Bratasz[2] [1]Jagiellonian University, Faculty of Chemistry, [2]Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences
13:55-14:05		**Visualization of Intermolecular Hydrogen Bonding of Poly(□-caprolactone) during Marine Degradation using Low-frequency Raman Spectroscopy** Harumi Sato[1], Tomoaki Segawa[1], Kohei Ito[1], Yota Maruyama[1], Masahiro Hatayama[1], Gao Jiacheng[1] [1]Kobe University
14:10-14:20		**Imaging of Three-dimensional Molecular Orientation Using FT-IR, Raman, and O-PTIR Microspectroscopies of various samples** Tomasz Wrobel[1] [1]Jagiellonian University
	A0-03	***(D) Spectroscopy of surface&interfaces*** Chair: Ahmad Salman
13:10-13:25		**Quantifying Large-Scale Structural Changes During pH-Induced Channel Opening of Influenza A M2 using Surface-enhanced Infrared Absorption Spectroscopy** Ronja Paschke[1], Swantje Mohr[2], Sascha Lange[2], Adam Lange[2], Jacek Kozuch[1] [1]Freie Universität Berlin [2]Leibniz-Forschungsinstitut für Molekulare Pharmakologie Berlin
13:30-13:45		**Mechanistic insights into the electrosynthesis of chemical feedstocks by in situ Raman and ATR-FTIR spectro-electrochemistry** Dr. Khoa H. Ly[1] [1]Fakultät für Chemie und Lebensmittelchemie, Technische Universität Dresden, Andreas-Schuber-t-Bau, Zellescher Weg 19, 01069 Dresden, Germany
13:50-14:00		**Nanoscale hyperspectral imaging of biologically relevant molecules** Ewelina Lipiec[1], Michał Czaja[2], Anna Chachaj-Brekiesz[3], Adrian Cernescu[4], Dhiman Ghosh[3], Dawid Lupa[1], Roland Riek[3], Sara Seweryn[2], Katarzyna Skirlińska-Nosek[2], Kamila Sofińska[1], Anita Wnętrzak[3], Marek Szymoński[1] [1]Jagiellonian University, Faculty of Physics, Astronomy, and Applied Computer Science, M. Smoluchowski Institute of Physics, Cracow, Poland [2]1) Jagiellonian University, Faculty of Physics, Astronomy, and Applied Computer Science, M. Smoluchowski Institute of Physics, Cracow, Poland, 2) Jagiellonian University, Doctoral School of Exact and Natural Sciences, Cracow, Poland [3]Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Kraków, Poland [4]Attocube Systems AG, Ellinger Weg 2, 85540 Haar, Germany

14:05-14:15		**Nanospectroscopy imaging of the molecule/metal interaction** Natalia Piergies[1], Dominika Święch[2], Magdalena Oćwieja[3], Czesława Paluszkiewicz[1], Wojciech M. Kwiatek[1] [1]Institute of Nuclear Physics Polish Academy of Sciences [2]AGH University of Science and Technology, Faculty of Foundry Engineering [3]Jerzy Haber Institute of Catalysis and Surface Chemistry Polish Academy of Sciences
	A0-01	***(H) Biodiagnostic spectroscopy*** Chair: Josep Sule-Suso
13:10-13:20		**Study on the effects of cryoconservation on human platelets** Diana E. Bedolla[1], Gaia Gavioli[2], Agnese Razzoli[2], Eleonora Quartieri[3], Barbara Iotti[3], Pamela Berni[3], Giovanni Birarda[4], Lisa Vaccari[4], Davide Schiroli[3], Chiara Marraccini[3], Roberto Baricchi[3], Lucia Merolle[3] [1]Area Science Park [2]Clinical and Experimental PhD Program, University of Modena and Reggio Emilia [3]AUSL-IRCCS di Reggio Emilia, Transfusion Medicine Unit [4]Elettra Sincrotrone Trieste
13:25-13:35		**Fighting peripheral nervous system tumors-hyperspectral imaging as a novel approach to monitor the therapeutic efficacy of cannabidiol** Karolina Chrabąszcz[1], Katarzyna Pogoda[1], Klaudia Suchy[1], Agnieszka Panek[1], Czesława Paluszkiewicz[1], Wojciech M. Kwiatek[1] [1]Institute of Nuclear Physics, Polish Academy of Science, Krakow, Poland
13:40-13:50		**Infrared tissue analysis of Hirschsprung's disease** Cymoril Combescot[1], Anne Durlach[2], Valérie Untereiner[3], Francesco Laconi[2], Olivier Piot[1] [1]University of Reims Champagne Ardenne, BioSpecT [2]Reims University Hospital [3]University of Reims Champagne Ardenne, Cellular and Tissular Imaging
13:55-14:05		**Infrared spectral biomarkers of neurodegenerative diseases** Lila Lovergne[1], Dhruba Ghosh[2], Renaud Schuck[1], Aris Polyzos[1], Michael Martin[3], Edward Barnard[4], James Brown[5], Cynthia McMurray[1] [1]Lawrence Berkeley National Laboratory/ Division of Molecular Biophysics and Integrated Bioimaging [2]Lawrence Berkeley National Laboratory/ Department of Statistics [3]Lawrence Berkeley National Laboratory/ Advanced Light Source [4]Lawrence Berkeley National Laboratory/ Molecular Foundry [5]Lawrence Berkeley National Laboratory/ Department of Statistics, and Division of Environmental Genomics and Systems Biology
14:10-14:20		**Multimodal spectroscopic imaging of cervical cancer cells exposed to the adaptogenic drug** Ewa Pięta[1], Katarzyna Pogoda[1], Klaudia Suchy[1], Karolina Chrabąszcz[1], Czesława Paluszkiewicz[1], Wojciech Kwiatek[1] [1]Institute of Nuclear Physics Polish Academy of Sciences
14:25-14:35		**FTIR imaging of kidney tissues to diagnose hypertensive organ damage and pharmacological treatment** Paola Sassi[1], Leonardo Pioppi[1], Niki Tombolesi[1], Reza Parvan[2], Gustavo Da Silva[2], Raffaele Altara[3], Marco Paolantoni[1], Assunta Morresi[1], Alessandro Cataliotti[2] [1]University of Perugia [2]University of Oslo [3]Maastricht University
14:45-15:00	A0-01	SHIM-POL presentation **Titel: Nice to have two features in one – the new AIRsight** **Subject: First measurement results obtained with the new AIRsight. The unique FTIR and Raman Microscope.**
18:30 (assembly 17:30)		**Conference Dinner**

Friday		
9:00-10:15	**A0-01**	**Plenary Session**
		Chair: Alexandre Brolo
9:00-9:30		**Molecular Optomechanics Approach to Surface-Enhanced Raman Scattering** Javier Aizpurua[1] [1]Center for Materials Physics (CSIC-UPV/EHU)
		Chair: Katarzyna Marzec
9:40-10:10		**Increasing the utility of infrared spectroscopic imaging by high performance instrumentation and AI** Rohit Bhargava[1] [1]Departments of Bioengineering, Electrical & Computer Engineering, Mechanical Science & Engineering, Chemical and Biomolecular Engineering, and Chemistry, Beckman Institute for Advanced Science and Technology, Cancer Center at Illinois, University of Illinois at Urbana--Champaign, 405 N. Mathews Ave., Urbana, IL 61801 USA
10:15-10:45		**Coffee Break**
10:45-12:10		**SESSION 1**
	A1-01	***(I) Chemometrics&machine learning*** Chair: Milda Pucetaite
10:45-11:00		**In silico experimentation to guide optimization and experimental design in clinical spectroscopy.** David Perez-Guaita[1], Victor Navarro-Esteve[1], Jaume Bejar-Grimalt[1], Angel Sanchez-Illana[1], Hugh J. Byrne[2] [1]University of Valencia [2]Technological University Dublin
11:05-11:20		**Sparse Wavelength Sampling in Mid-Infrared Spectroscopy** Valeria Tafintseva[1], Miriam Aledda[1], Boris Zimmermann[1], Nageshvar Patel[1], Volha Shapaval[1], Achim Kohler[1] [1]Norwegian University of Life Sciences
11:25-11:35		**Green Pharmaceutical Quality Control via Infrared Spectroscopy** Silke Lehner[1], Mona Tawab[2], Holger Latsch[2], Sandra Ganß[2], Boris Mizaikoff[3], Robert Stach[1] [1]Hahn-Schickard [2]Zentrallaboratorium-Deutscher Apotheker [3]Hahn-Schickard
11:40-11:50		**Influence of Infrared Imaging measurement modes on breast tissue recognition and cancer diagnosis** Danuta Liberda[1], Tomasz P. Wróbel[2] [1] Jagiellonian University, Doctoral School of Exact and Natural Sciences, Prof. St. Łojasiewicza 11, PL30348, Cracow, Poland 2 Solaris National Synchrotron Radiation Centre, Jagiellonian University, Czerwone Maki 98, 30-92 Krakow, Poland [2]2 Solaris National Synchrotron Radiation Centre, Jagiellonian University, Czerwone Maki 98, 30-92 Krakow, Poland
11:55-12:05		**Infrared Diffraction Microtomography of Biological Samples by Solving the Inverse Scatter Problem** Eirik Almklov Magnussen[1], Boris Zimmermann[1], Uladzislau Blazkho[1], Simona Dzurendova[1], Benjamin Dupuy-Galet[1], Dana Byrtusova[1], Florian Muthreich[2], Valeria Tafintseva[1], Kristian Hovde Liland[1], Volha Shapaval[1], Achim Kohler[1] [1]Norwegian University of Life Sciences [2]University of Bergen
	A1-02	***(J) Computational approaches*** Chair: Thomas Mayerhöfer
10:45-10:55		**Computing Raman and Raman optical activity spectra for molecules under resonance** James Cheeseman[1] [1]Gaussian, Inc.
11:00-11:10		**Yes we can! Calculational study of Human Serum Transferrin distinguishes between resonance Raman optical activity and circularly polarized Raman** Jonathan Bogaerts[1], James Cheeseman[2], Wouter Herrebout[1], Christian Johannessen[1] [1]University of Antwerp [2]Gaussian Inc.
11:15-11:25		**Simulation of vibrational spectroscopies in various environments** Vincent Liegeois[1] [1]NISM, Unamur

11:30-11:40		**Anharmonicity of amide bands in NIR region – overtones, combinations, structural fingerprint of peptides** Justyna Grabska[1], Krzysztof B. Bec[1], Christian W. Huck[1] [1]University of Innsbruck
11:45-11:55		**Resonance Raman Optical Activity: how to properly measure, correct and simulate spectra** Grzegorz Zając[1], Ewa Machalska[2], Katarzyna Pajor[3], Josef Kapitán[4], Petr Bouř[5], Malgorzata Baranska[6] [1]Jagiellonian Centre for Experimental Therapeutics (JCET), Jagiellonian University [2]Jagiellonian Centre for Experimental Therapeutics (JCET), Jagiellonian University; Institute of Nuclear Chemistry and Technology [3]Faculty of Chemistry, Jagiellonian University [4]Department of Optics, Palacký University Olomouc [5]Institute of Organic Chemistry and Biochemistry, Academy of Sciences [6]Faculty of Chemistry, Jagiellonian University; Jagiellonian Centre for Experimental Therapeutics (JCET), Jagiellonian University
	A0-04	***(A) Advanced characterization of materials*** Chair: Sagie Katz
10:45-11:00		**Operando IR spectroscopic investigations of (hybrid) porous materials** Marco Daturi[1] [1]Laboratory of Catalysis and Spectrochemistry, ENSICAEN, UNICAEN, CNRS
11:05-11:20		**In situ FTIR, RS and coupled RS/AFM methods for surface understanding of metal oxide materials applied as catalysts for methane abatement** Joanna Profic-Paczkowska[1] [1]Faculty of Chemistry Jagiellonian University
11:25-11:35		**Structural characterization of amorphous silica coatings combining specular reflectance (SR) and attenuated total reflectance (ATR) infrared spectroscopic techniques** Brenda Bracco[1], Helios Vocca[2], Silvia Corezzi[2], Alessandro Di Michele[2], Laura Silenzi[3], Angela Trapananti[3], Flavio Travasso[3], Stefano Colace[4], Michele Magnozzi[5], Paola Sassi[1] [1]Department of Chemistry, Biology and Biotechnology, University of Perugia and Istituto Nazionale di Fisica Nucleare, Sezione di Perugia [2]Department of Physics and Geology, University of Perugia and Istituto Nazionale di Fisica Nucleare, Sezione di Perugia [3]School of Science and Technology – Physics Division, University of Camerino and Istituto Nazionale di Fisica Nucleare, Sezione di Perugia [4]Department of Physics, Università di Genova [5]Department of Physics, Università di Genova, and Istituto Nazionale di Fisica Nucleare, Sezione di Genova
11:40-11:50		**Can elevated temperatures in HTGR nuclear reactors reverse irradiation damage in graphite? – high-temperature in-situ Raman spectroscopy study** Magdalena Gawęda[1], Piotr Jeleń[2], Małgorzata Frelek-Kozak[1], Łukasz Kurpaska[1], Jacek Jagielski[3] [1]NOMATEN CoE, NOMATEN MAB, National Centre for Nuclear Research [2]AGH University of Science and Technology [3]National Centre for Nuclear Research, Łukasiewicz Institute for Microelectronics & Photonics
	A0-03	***(D) Spectroscopy of surface&interfaces*** Chair: Cecilia Spedalieri
10:45-11:00		**Surface-enhanced Raman Scattering in scaffolds for 3D cell cultures** Judith Langer[1], Javier Plou[2], Clara Clara García-Astrain[1], Beatriz Molina-Martínez[3], Luis M. Liz-Marzán[4] [1](1) CIC biomaGUNE, Basque Research and Technology Alliance (BRTA), (2) Biomedical Research Networking Center in Bioengineering, Biomaterials, and Nanomedicine (CIBER-BBN) [2](1) CIC biomaGUNE, Basque Research and Technology Alliance (BRTA), (2) Biomedical Research Networking Center in Bioengineering, Biomaterials, and Nanomedicine (CIBER-BBN), (3) CIC bioGUNE, Basque Research and Technology Alliance (BRTA) [3](1) CIC biomaGUNE, Basque Research and Technology Alliance (BRTA) [4](1) CIC biomaGUNE, Basque Research and Technology Alliance (BRTA), (2) Biomedical Research Networking Center in Bioengineering, Biomaterials, and Nanomedicine (CIBER-BBN), (4) IKER-BASQUE, Basque Foundation for Science
11:05-11:15		**Spectroscopic study of extracellular vesicles using plasmonic nanoobjects** Tímea Bebesi[1], Marcell Pálmai[1], Anikó Gaál[1], Imola Csilla Szigyarto[1], Orsolya Bálint-Hakkel[2], Zoltán Varga[1], Judith Mihály[1] [1]Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences [2]Institute of Technical Physics and Material Sciences, Centre for Energy Research

11:20-11:30		**Giant plasma membrane vesicles as the model systems to resolve nanoscale heterogeneity of native lipid membranes** Katarzyna Pogoda[1], Klemencja Berghauzen-Maciejewska[2], Natalia Piergies[2], Karolina Chrabąszcz[2], Czesława Paluszkiewicz[2], Wojciech Kwiatek[2] [1]Institute of Nuclear Physics Polish Academy of Sciences [2]Institute of Nuclear Physics PAN
11:35-11:45		**SERS based detection of cytosine methylation in genomic DNA** Stefania D. Iancu[1], Vlad Moisoiu[1], Adrian B. Tigu[2], Andrei Stefancu[1], Zoltán Bálint[1], Ciprian Tomuleasa[2], Nicolae Leopold[1] [1]Faculty of Physics, Babeș-Bolyai University [2]Medfuture Research Center for Advanced Medicine, Iuliu Hatieganu University of Medicine and Pharmacy
	A0-01	***(H) Biodiagnostic spectroscopy*** Chair: Bayden Wood
10:45-11:00		**Finding a Needle in a Haystack: Transmission Raman Spectroscopy (TRS) for Detecting Micro Calcifications in Breast Tissue** Benjamin Gardner[1], Jennifer Haskell[1], Adrian Ghita[2], Charlotte Ives[3], Douglas Ferguson[3], Pavel Matousek[4], Nick Stone[1] [1]Univeristy of Exeter [2]University of Hertfordshire [3]Royal Devon University Healthcare NHS Foundation Trust [4]STFC
11:05-11:15		**SERS analysis of urine for prostate cancer detection** Nicolae Leopold[1], Stefania D. Iancu[1], Andrei Stefancu[1], Vlad Moisoiu[1], Teodora Telecan[2], Iulia Andras[2], Nicolae Crisan[2] [1]Faculty of Physics, Babeș-Bolyai University [2]Urology Department, Iuliu Hatieganu University of Medicine and Pharmacy
11:20-11:30		**Vibrational spectroscopy for differential diagnosis of patients with rheumatoid and psoriatic arthritis** Sylwester Mazurek[1], Izabela Kokot[2], Agnieszka Piwowar[2], Renata Sokolik[2], Monika Kacperczyk[2], Kamil Rodak[2], Roman Szostak[1], Lucyna Korman[2], Ewa Kratz[2] [1]University of Wroclaw, Department of Chemistry [2]Wroclaw Medical University
11:35-11:45		**Infrared spectroscopy for rapid and objective diagnosis of the etiology of infection as bacterial or viral using a simple peripheral blood test.** Ahmad Salman[1], Uraib Sharaha[2], Guy Beck[3], Yotam D. Eshel[3], Gal Cohen-Logasi[4], Adam H. Agbaria[5], Itshak Lapidot[6], Joesph Kapelushnik[3], Mahmoud Huleihel[2], Shaul Mordechai[5] [1]SCE-Sami Shamoon College of Engineering/ Department of Physics [2]Ben-Gurion University/Department of Microbiology, Immunology, and Genetics [3]Soroka University Medical Center/Department of Hematology and Oncology, Saban Pediatric Medical Center [4]SCE-Sami Shamoon College of Engineering/Department of Green Engineering [5]Ben-Gurion University, Department of Physics [6]Afeka Tel-Aviv Academic College of Engineering, Department of Electrical and Electronics Engineering
12:10-12:45	**A0-01**	**Award&Closing Ceremony**
12:10-12:20		ICAVS Awards
12:20-12:30		Introduction of ICAVS 13
12:30-12:45		Summary of ICAVS 12 and Good Bye
12:45-13:45		**Lunch**