Greetings from the conference chairs!

The Faculty of Chemistry at Jagiellonian University in Krakow is proud to have been entrusted with hosting the twelve International Conference on Advanced Vibrational Spectroscopy (ICAVS12). It is our pleasure to have you here with us, especially after the difficult time of the Covid-19 pandemic when ICAVS11 was organised virtually. We hope that you will find this conference informative, engaging, and valuable. Our goal is to provide you with a platform to learn and share knowledge with other professionals in your field.

The ICAVS Conference Series aims to bring together researchers, application scientists, and instrumentation developers from universities, research institutes, and industry. It focuses on all disciplines of vibrational spectroscopy, mid- and near-infrared, Raman as well as non-linear effects, pushing limits of molecular detection to single molecules and nanoscale. ICAVS12 will maintain that tradition of combining cutting-edge fundamental and technological advances with a rich social program in the relaxing atmosphere of the Royal City of Krakow.

For the first time in the ICAVS history, the Steering Committee has established two ICAVS awards – ICAVS Award for Outstanding Achievements and ICAVS Young Scientist Award. These awards aim to honor prominent researchers, who actively participate at ICAVS conferences, for their significant contributions and notable achievements in instrumentation and methods developments in the field of vibrational spectroscopy.

We thank the 450+ scientists from over 30 countries for accepting our invitation, their interest and participation as well as the national institutions and the exhibiting and sponsoring companies for their support. The Marshal of the Malopolska province, the Mayor of Krakow, the Rector of Jagiellonian University, as well as Polish Chemical Society, are honoured to host and support this exceptional scientific conference wishing you an enjoyable meeting filled with new knowledge, friendship, and memories.

We look forward to meeting and interacting with you all at ICAVS12, a great place to grow, stimulate academic development, and broaden the horizons of the applications of vibrational spectroscopy in science.

Conference Chair
Kamilla Małek
Jagiellonian University in Kraków

Conference Co-Chair
Katarzyna Majzner
Jagiellonian University in Kraków

Program Chair
Janina Kneipp
Humboldt-Universität zu Berlin

Program Co-Chair
Małgorzata Baranska
Jagiellonian University in Kraków
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Organizers

Jagiellonian University in Krakow

Raman Imaging Group Faculty of Chemistry

The International Society for Clinical Spectroscopy

Targi w Krakowie Ltd.
Committees

Program Committee

Halina Abramczyk ................................................................. Poland
Freek Ariese ................................................................. Netherlands
Claudia Beleites ................................................................. Germany
Ewan Blanch ................................................................. Australia
Mischa Bonn ................................................................. Germany
Hugh Byrne ................................................................. Ireland
Jon Camden ................................................................. USA
Zhenchao Dong ................................................................. China
Barbara Gil ................................................................. Poland
Kathleen M. Gough ........................................................ Canada
Hiro-o Hamaguchi ................................................................. Japan
Alison Hobro ................................................................. Japan
Natalia Ivleva ................................................................. Germany
Young Mee Jung ................................................................. South Korea
Judy Kim ................................................................. USA
Achim Kohler ................................................................. Norway
Wojciech Kwiatek ................................................................. Poland
Igor Lednev ................................................................. USA
Jian-Feng Li ................................................................. China
Marena Manley ................................................................. South Africa
Mike Martin ................................................................. USA
Lisa Miller ................................................................. USA
Wei Min ................................................................. USA
Chadrabas Narayana .............................................................. India
Michele Ortolani ............................................................... Italy
Yukihiro Ozaki ................................................................. Japan
Isabela Pastoriza-Santoz ........................................................ Spain
Gerwin Puppels ............................................................. Netherlands
Dario Polli ................................................................. Italy
Jürgen Popp ................................................................. Germany
Vinod K. Rastogi .............................................................. India
Harumi Sato ................................................................. Japan
Frederike Vanholsbeeck ...................................................... New Zealand
Yuling Wang ................................................................. Australia
Inez Weidinger ................................................................. Germany
International Steering Committee

Chair of Steering Committee:
Alexandre Brolo ................................................................. Canada ........................................................................ (until 2023)

Secretary of Steering Committee:
Dennis Hore ........................................................................ Canada ........................................................................ (until 2023)
Keith Gordon ........................................................................ New Zealand ................................................................ (until 2025)
Ian Lewis .............................................................................. USA ........................................................................ (until 2025)
Małgorzata Baranska ......................................................... Poland ........................................................................ (until 2027)
Sergei Kazarian ................................................................. UK ........................................................................ (until 2027)
Kamilla Malek ...................................................................... Poland ........................................................................ (until 2029)
Janina Kneipp ...................................................................... Germany ...................................................................... (until 2029)
Bin Ren .............................................................................. China ........................................................................ (until 2031)
Hongfei Wang ................................................................ China ........................................................................ (until 2031)

International Steering Committee
Kamilla Malek
Małgorzata Baranska
Katarzyna Majzner
Anna Antolak
Aleksandra Borek-Dorosz
Jakub Dybas
Anna Nowakowska
Ewa Machalska
Sylwia Orzechowska
Szymon Tott
Adrianna Wisłocka-Orlowska
Grzegorz Zajac

CLIRSPEC Representatives
Hugh Byrne ........................................................................ Ireland
Alex Henderson ................................................................ UK
Jagiellonian University in Kraków

The Jagiellonian University is the oldest higher education institution in Poland and one of the oldest in Europe. It was founded on 12 May 1364 by the Polish king Casimir the Great. The Studium Generale, as the University was then called, comprised three faculties of liberal arts, medicine, and law. The oldest, main college was at first called the Royal Jagiellonian College (Collegium Regium), and then the Greater College (Collegium Maius), now the University Museum. The University, located in the capital of the Kingdom of Poland, never again interrupted its educational and scholarly activity. Not only does it constitute a symbol of the continuity of the Polish state, but also places Krakow among the most important educational center in the country.

The University is a place where Nicolaus Copernicus and Karol Wojtyla, the future Pope John Paul II, were world-famous scholars, and Karol Olszewski and Zygmunt Wroblewski liquefied oxygen and nitrogen. In 2016, Prof. Yukihiro Ozaki was distinguished by the JU honorary doctorate. Jagiellonian University has been an international scientific unit since its very beginning. Poles, Ruthenians, Lithuanians, Hungarians, Germans, Czechs, Swiss, English, Dutch, French, Spanish, Italians, and even Tatars studied here in the old days.

Today the University employs 3.8 thousand academic staff, including over 650 professors, as well as about 3.5 thousand other staff members, while providing education to about 40 thousand students. Currently, Jagiellonian University comprises 16 faculties, including the Medical College. Large-scale investments financed the Campus of the 600th Anniversary of the Jagiellonian University Revival, where the Faculty of Chemistry, Faculty of Physics, Astronomy and Applied Computer Science, Centre for Natural Sciences Education, Synchrotron SOLARIS, and others have been recently relocated.

Today, Jagiellonian University is involved in various international cooperation activities, including research and educational projects, faculty and student exchanges within bilateral agreements, Erasmus+ and SYLFF, summer schools, networks, innovation, and technology transfer as well as different scholarship schemes, during which young researchers pursue their academic interests and develop friendships with people who share their passion. The eminent researchers and state-of-the-art infrastructure make the UJ one of the leading Polish scientific institutions that also is widely recognized through research achievements. Jagiellonian University is invariably ranked as one of the top universities in Poland. As one of very few Polish higher education institutions, it is frequently featured on the most important international ranking lists, e.g., QS World University Ranking, Shanghai Ranking, and Center for World University Rankings (CWUR).
Yet another advantage of Jagiellonian University is its location in the historic city of Kraków, the former capital of Poland and a great cultural center, visited by millions of tourists. Some of the University buildings are major historical sites themselves. A part of the University, Jagiellonian University Campus 600th anniversary of the Renewal, is also located in the Ruczaj District, where the life sciences departments are located.
The Faculty of Chemistry of the Jagiellonian University was formally transformed from the Institute of Chemistry in 1981. The history of chemistry at Jagiellonian University dates back to the 18th century when the Department of Chemistry and Natural History was located at the Faculty of Medicine. In 2017, the Faculty was relocated to the Campus of the 600th Anniversary of the Revival of the Jagiellonian University. Since 2013, the Faculty of Chemistry has been continuously ranked among Poland's best scientific and research units. It has the A+ scientific category awarded by the Ministry of Science and Education. Research conducted by scientists from the JU Faculty of Chemistry is appreciated and rewarded for quality and innovation. The Faculty of Chemistry is one of the most active faculties in the field of patenting and commercializing research results, contributing to the success of the entire university, which for several years has been considered the most innovative university in Central and Eastern Europe. The Faculty has the most extensive base of various chemical equipment in the Lesser Poland (Malopolska) province, several specialized laboratories with the highest standards, where scientific research in chemical technology, catalysis, electrochemistry, and medical chemistry is carried out. Recently, the Faculties of Chemistry and Physics received a grant of EUR 25 million to develop the Center for Materials Research at the Atom Scale for the INnovative Economy (ATOMIN). The Faculty offers modern study programs in Chemistry, Environmental Chemistry, Medical Chemistry, Chemistry of Sustainable Development, and Advanced Spectroscopy in Chemistry, which are ranked in 1st place in Poland. The Doctoral School in Chemical Sciences has been educating over 100 PhD students.
CLIRSPEC

Over the years, spectroscopy has become a successful and well-established tool in the investigation of cells, tissues, and other biological materials. This has driven efforts to translate spectroscopy into the fields of clinical and pharmacological applications. In order to help coordinate efforts globally, the International Society for Clinical Spectroscopy (CLIRSPEC, https://clirspec.org/) was established, as a non-profit organization, in 2015. CLIRSPEC is the platform for individual researchers, teams, and organizations wishing to promote new solutions for clinicians to improve patient diagnosis and disease prognosis. CLIRSPEC welcomes anyone interested in the translation of molecular spectroscopic techniques, in particular infrared and Raman spectroscopy, into the clinical arena.

Conference Secretariat

Targi w Krakowie Ltd. is the largest organizer of conferences, congresses, and fairs in the south of Poland and the third in the country. The company has been organizing the most important industry events for over 27 years. We are proudly a member of ICCA and UFI.

Targi w Krakowie Ltd.
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31-586 Krakow
http://kongresy.krakow.pl
Phone: +48 12 651 90 71, +48 12 651 95 42
Email: icavs2023@targi.krakow.pl
Honorary Patronage

Witold Kozłowski
The Marshal
of the Małopolska Region

Jacek Majchrowski
The Mayor
of the City of Krakow

Prof. dr. hab. Jacek Popiel
The Rector of the Jagiellonian
University in Krakow

The Polish
Chemical Society
History of ICAVS

ICAVS Conferences have a well-established tradition and rich history. However, the beginning of the ICAVS meetings dates back to the 70s and stemmed from two other conferences: the International Conference on Fourier Transform Spectroscopy (ICOFTS) and the Advanced Infrared Spectroscopy (AIRS). The first one, ICOFTS, began in 1970 in Aspen, USA and continued in 1977 and 1981 in South Carolina, USA. Following 1981, ICOFTS became a biennial conference. The first meeting outside the USA was held in Durham, UK and meetings continued to run at locations around the globe. The latter, AIRS, had its beginning in 1993 in Tokyo, Japan as a special conference and was originally not intended to be a series. However, the next AIRS meetings took place in North Carolina, USA (1996) and Vienna, Austria (1998). Both conferences helped to shape the present form of the ICAVS conference.

In the late 1990s, to bring scientists together it was decided to join these meetings and establish one conference entitled the International Conference on Advanced Vibrational Spectroscopy (ICAVS). The first one of the ICAVS meetings was held in 2001 in Turku, Finland and continues as a biennial conference moving throughout the world. The ICAVS conference rotates among the continents, with ICAVS7 held in Japan (2013), ICAVS8 in Austria (2015), ICAVS9 in Canada (2017) and ICAVS10 in New Zealand (2019), and ICAVS11 in Poland (2021, online).

Each ICAVS event gathers between 450-700 participants from all over the world, including UK, Australia, New Zealand, South Korea, Poland, India, Austria, Canada, USA, Germany, Japan, France, China and Brazil.
<table>
<thead>
<tr>
<th>CONFERENCE</th>
<th>YEAR</th>
<th>LOCATION</th>
<th>CHAIR</th>
<th>PROGRAM CHAIR</th>
</tr>
</thead>
<tbody>
<tr>
<td>ICAVS1</td>
<td>2001</td>
<td>Turku, Finland</td>
<td>Jyrki Kauppinnen</td>
<td>Matti Hotokka</td>
</tr>
<tr>
<td>ICAVS2</td>
<td>2003</td>
<td>Nottingham, UK</td>
<td>Michael George</td>
<td>John Chalmers</td>
</tr>
<tr>
<td>ICAVS3</td>
<td>2005</td>
<td>Wisconsin, USA</td>
<td>Larry Nafie and Rina Dukor</td>
<td></td>
</tr>
<tr>
<td>ICAVS4</td>
<td>2007</td>
<td>Corfu, Greece</td>
<td>Vasilius Gregariou</td>
<td>Bernhard Lendl</td>
</tr>
<tr>
<td>ICAVS5</td>
<td>2009</td>
<td>Melbourne, Australia</td>
<td>Donald McNaughton</td>
<td>Bayden Wood</td>
</tr>
<tr>
<td>ICAVS6</td>
<td>2011</td>
<td>California, USA</td>
<td>James de Haseth</td>
<td>Curtis Marcott</td>
</tr>
<tr>
<td>ICAVS7</td>
<td>2013</td>
<td>Kobe, Japan</td>
<td>Yukihiro Ozaki</td>
<td>Taskeshi Hasegawa</td>
</tr>
<tr>
<td>ICAVS8</td>
<td>2015</td>
<td>Vienna, Austria</td>
<td>Bernhard Lendl</td>
<td>Michael George</td>
</tr>
<tr>
<td>ICAVS9</td>
<td>2017</td>
<td>Victoria, Canada</td>
<td>Alexandre Brolo</td>
<td>Dennis Hore</td>
</tr>
<tr>
<td>ICAVS10</td>
<td>2019</td>
<td>Auckland, New Zealand</td>
<td>Keith Gordon and Frédérique Vanholsbeeck</td>
<td>Ian R. Lewis and Cushla McGoverin</td>
</tr>
<tr>
<td>ICAVS11</td>
<td>2021</td>
<td>Krakow, Poland</td>
<td>Malgorzata Baranska, Kamilla Malek and Katarzyna M. Marzec</td>
<td>Sergei Kazarian</td>
</tr>
<tr>
<td>ICAVS12</td>
<td>2023</td>
<td>Krakow, Poland</td>
<td>Kamilla Malek, Malgorzata Baranska and Katarzyna Majzner</td>
<td>Janina Kneipp</td>
</tr>
</tbody>
</table>
Since 2001 the International Conference on Advanced Vibrational Spectroscopy (ICAVS) brings together leading researchers, applications scientists, clinicians, and engineers focused on advances in a wide range of spectroscopic techniques.

ICAVS 2023 is the 12th conference in the successful ICAVS series, providing a fresh unique occasion to discuss recent discoveries, new trends, and directions related mainly to infrared and Raman spectroscopies as well as to exchange knowledge and ideas in this field of science.

We made together every effort to create a remarkable program that continues tradition of inspiring scientific meetings. As previous, this year ICAVS is particularly focused on development of spectroscopic methods and their interdisciplinary applications. Conference program will span talks over 60 invited and 60 regular talks focused on cutting-edge science. The line-up of ten plenary speakers includes experts from United Kingdom, Switzerland, Germany, Poland, China, Japan, USA, Canada, and Australia.

A special session – Perspective Lectures – is led by four prominent scientists and summaries the current developments in their research fields with future perspectives for fundamental techniques of infrared and Raman spectroscopy. This global event also offers an opportunity for scientific discussion and finding solutions to current challenges in the field of vibrational spectroscopy.

Among the perspectives, plenary, and invited speakers, there are scientists from 27 countries around the world. It is worth noting that among the conference speakers, women have a significant contribution and constitute 43% and 40% of the invited and plenary speakers, respectively.
General Information about Poland and Kraków

About Poland:

Capital: Warsaw
Language: Polish
Currency: złoty (PLN, zł)
Population: 38 million
Area: 322,575 sq km (124,547 sq miles)
Time Zone: CET (UTC+1)

Climate in August: This is the second hottest month of the year and one of the best times to visit Krakow. Temperatures are usually in the high teens and often reach up to 24°C on a hot day. Evenings are chilly, ca. 15°C. August is relatively dry.

Government type: Republic, parliamentary democracy
Members of: EU, UN, NATO, OECD, WTO, and many other
Country Code: PL

Electricity
230V AC electricity. Power outlets are usually two-prong round sockets. To avoid the hassle of having to buy new adaptors everywhere you go, we recommend picking up a Universal Travel Adaptor before you leave.

Currency
The national currency in Poland is złoty (PLN/zł) divided into 100 groszy. Coins come in 1, 2, 5, 10, 20, and 50 groszy, as well as 1, 2, and 5 złoty, while banknotes’ denominations note as 10, 20, 50, 100, 200 and 500 złoty. The odd hotels or restaurants may accept euros or dollars but ATMs and exchange counters can be found throughout the country, thus you will not have a problem getting local currency.

Language
Polish is a native and the official language in Poland. Although not a native language, English is one of the most common languages that are learned and spoken in Poland. It is taught in schools and almost anyone working in the tourism industry in a big city speaks English.

Kraków
Due to its demographic, economic, social, and scientific-cultural strength – ranks second in Poland among cities. It has high-quality human capital at its disposal. Krakow is a city which people consciously choose as a place to live, work, study, and spend free time in a variety of ways. Sustainable development and the ability to meet specific challenges with the skillful use of own resources are the main priorities.

The academic center is permanently connected with the city and builds an unrepeated resource of knowledge in a unique way. It is the key to competitiveness and innovation not only of Krakow, but also of the entire region. The intensively developing economy based on knowledge, which is a completely new process in the economic life of the city, makes it a part of the modern economies of the world.

The overriding goal for Krakow is not only to be a modern city, but also to be proud of its historical heritage. It aspires to be an open, rich, friendly, and safe metropolis, vibrant with culture. The research and development sectors are the foundations for the development of Krakow – a city where innovation and effective cooperation between science and business are the focus.

Information about sightseeing, culture, and current events is available on the official Krakow website: www.krakow.pl/english/
Emergency Information

112 is the European emergency phone number, available everywhere in the EU, free of charge. You can call 112 from fixed and mobile phones to contact any emergency service: an ambulance, the fire brigade, or the police. In Poland 112 calls are answered by the Fire Brigade and Police.

+48 12 999: Ambulance
998: Fire brigade
997: Police
981: Emergency Road Service
986: Municipal police

If you are using a mobile/cellular phone: remember to dial the local code before the direct emergency number; for example: 12 + 997 to call the police in Kraków.

If you do not know the local code, dial the general emergency number: **112** and the operator will request the appropriate emergency unit.

Tourist Emergency Helpline – While in Poland, are you experiencing difficulties? Have you lost your passport, are you in need of medical help or road assistance but you are not sure whom to contact in an emergency?

+48 222 787 777, +48 608 599 999

Numbers which may be also be useful:

Krakow public transportation information – Information on timetables, transport connections, current transport conditions, tickets, items lost in vehicles, and complaints regarding the Kraków City Card and ticket vending machines.

12 19 150

KRK Airport Information 24h: +48 12 295 58 00
0 801 055 000 (only landline)

InfoKraków tourist information – tourist information provides detailed information on accommodation (including hotel reservations) and travel products, tourist attractions in Krakow and the region (sales of maps, guidebooks), concerts and cultural events in Krakow, transfers from the airport to the tourist’s final destination in Malopolska.

48 12 285 53 41

Public Transport

You can take advantage of many local transportation systems in Krakow, such as buses and a wide net of trams. In the very city center, there are plenty of tram and bus lines in service in Krakow that help you get around the city and go beyond its limits (e.g. to Wieliczka). Public transport is organized by the Municipal Infrastructure and Transport Board (ZIKiT) of Krakow. Maps of city transport lines are available on the website of the Municipal Transport Facility (Miejskie Przedsiębiorstwo Komunikacyjne, MPK – www.mpk.krakow.pl), and the timetables can be found on its website and at individual stops.

Finding your connection: [krakow.jakdojade.pl](http://krakow.jakdojade.pl)

On Sundays and holidays of the summer season, vintage trams travel the streets of Kraków. More information: [www.muzealna.org](http://www.muzealna.org)
Map of tram lines

Map of buses and trams
Train system and tram+bus system operate on different tickets. Train tickets for the SKA Koleje Małopolskie trains (Kraków Airport, Wieliczka directions) can be purchased at the stations in the ticket machines (cash, credit or debit card), eg. on the Krakow Airport station, as well as onboard the train from the train conductor (cash, credit or debit card). Train tickets are validated by the train conductor inside the train. A single ticket from the Kraków Airport to the Kraków Główny (Main Railway Station) costs 17 PLN. For more information about train transportation please visit krakowairport.pl, and kolejemalopolskie.com.pl.

Tram/bus tickets can be purchased at selected stops in the ticket machines (cash, credit/debit cards), inside the trams and buses in the ticket machines (coins, credit/debit cards) in the newspaper shops or using mobile apps, e.g., iMKA, mPay, moBiLET, SkyCash, jakdojade or zbiletem.pl. Paper tickets need to be validated onboard trams and buses. More information about the ticket system can be found here: ztp.krakow.pl

How to get to the city from the Kraków Airport

- To hotels near Rondo Grunwaldzkie and the Kazimierz district: bus 300 from the Kraków Airport stop (direction Os. Podwawelskie) to the Rondo Grundwaldzkie stop (5 stops, 22 min), 60 min – ticket: 6 PLN
- To hotels near the Main Square: SKA train from the Kraków Lotnisko stop to the Kraków Główny (Main Railway station) stop (6 stops, 17 min, cost 17 PLN)
- By taxi, it costs approximately 50-90 PLN, depending on the company, and takes approximately 15-20 min. Also ridesharing companies (e.g., Uber, Bolt) operate at the airport and in the city.
Registration & Information

Conference registration includes access to the entire conference program including Perspective Session, Opening and Closing Ceremony, Plenary Sessions and Oral Presentations, workshops of Companies, Poster Sessions, Coffee Breaks, Lunches, tickets for public transport in the city of Krakow valid for the entire duration of the conference. Additionally, access to the Conference Book (pdf), the Book of Abstract (pdf), and other conference materials is available online on the Conference website.

Accompanying person fee includes access to the Coffee Breaks, Lunches, Welcome Cocktail, and the organized city tour.

Registration and Information Desk Hours

The registration and information desk is located on the ground floor of the conference venue in front of the main entrance. Registration will start on Sunday, August 27 at 10:00. The conference desk will be staffed until 21:00 on Sunday, and from 8:00 through 18:00 on Monday, Wednesday. On Tuesday, Thursday and Friday opening hours of the conference desk will be 8:00 – 15:00. If you need assistance during the conference, please visit the Registration Desk.

Staff

ICAVS staff from Conference Management can be identified by color marking on their name badges. Feel free to ask anyone of our staff for assistance. For immediate assistance

Please visit us at the Registration Desk.

Conference Regulations

Your name badge is your admission ticket to the conference sessions, coffee breaks, reception, and social events. For security reasons, please always wear your ICAVS12 badge while on the conference premises.

Smoking is permitted only outside the conference venue. Photography and recording are not permitted in any oral or poster session.

We will have a small film team on location to cover ICAVS 12. If you do not wish to be filmed, please approach them and indicate so.

Venue

ICAVS 12 will take place in the Faculty of Chemistry Jagiellonian University (JU) in Krakow (Poland), located at the Campus of the 600th Anniversary of the JU Revival on Gronostajowa St. 2, Krakow, Poland.

The plenary and perspective lectures, as well as the opening and closing ceremony, will take place in lecture hall A0-01, which is located on the ground floor. The entrance to this lecture hall is from the ground and the first floor.

Invited and regular talks will take place in parallel sessions in the lecture halls A0-01, A0-03, A0-04, A1-01 and A1-02. Access to lecture halls A1-01 and A1-02 is from the first floor only.

Welcome Cocktail, poster sessions, coffee breaks, and lunches will be held in the exhibition area on the ground and first floor.
How to get to the venue from the city center:

Trams: 11, 17, 18, 52, 62 to the stop Ruczaj

- from hotels near the Kazimierz Distinct and Dietla street (Stradom, Orzeszkowej stops): tram 18, 52 (direction Czerwone Maki P+R) to the Ruczaj stop (10 stops, 16 min), 20 min-ticket: 4 PLN
- from hotels near the Rondo Grunwaldzkie stop: tram 18, 52 (direction Czerwone Maki P+R) to the Ruczaj stop (8 stops, 12 min), 20 min-ticket: 4 PLN
- from the Main Railway station,
  - tram line 17, from the Dworzec Główny Tunel stop (direction Czerwone Maki P+R) to the Ruczaj stop (19 stops, 32 min, 60 min – ticket: 6 PLN), usunac or
  - tram line 52, from the Teatr Słowackiego stop (direction Czerwone Maki P+R) to the Ruczaj stop (13 stops, 21 min, 60 min – ticket: 6 PLN)

Look on the map of the Kraków Główny (Main Railway Station) transportation, to locate tram stops.

- from the Main Square:
  - tram line 52, from the Poczta Główna (direction Czerwone Maki P+R) to the Ruczaj stop (12 stops, 20 min, cost 6 PLN)
  - tram line 18, from the Plac Wszystkich Świętych (direction Czerwone Maki P+R) to the Ruczaj stop (13 stops, 20 min, cost 6 PLN)

The timetable is available here:
rozklady.mpk.krakow.pl
jakdojade.pl/krakow

You can also download app Jak dojade

Description automatically generated on your mobile from Google and Apple stores

Participants will receive a 1-week ticket for public transport in Krakow at the conference desk. Ticket will be in the form of sticker on the Conference ID. Please remember to have your Conference ID every time you use tram or buses.

WiFi

WiFi connection is available throughout the conference venue. You will receive an access code during registration. EDUROAM network will be also available.
Social program

Welcome Cocktail
WHEN? 27.08 (Sunday) – 19:30-21:30
WHERE? Conference Venue
Sponsor: LABSOFT

Excursions
WHEN? 29.08 (Tuesday) – 15:00-18:00
WHERE? Meeting place: Conference Venue

Tour 1 – Hop on Hop off plus short walking tour – LIMITED TICKETS
The tour takes place on 29.08 (Tuesday) 15:00-18:00
The Hop on Hop off bus will show you old and new Krakow. You will see the most popular and characteris-
tic places and sights of Cracow e.g. old Podgórze and Zabłocie Districts, Schindler’s Factory. The tour also
includes a walk along the Royal Route from the Florian Gate to the Main Square and a visit to the stunning
St. Mary’s Church with its breathtaking altar by Veit Stoss.

Tour 2 – Medieval Cracow
The tour takes place on 29.08 (Tuesday) 15:00-18:00
The trip is addressed to people who like discovering the secrets of the city on foot. It includes visiting the
Wawel Hill with majestic Wawel Castle, the Old Town with the stunning St. Mary’s Church on the Main
Square and the old University quarter with Jagiellonian University Museum.

ALL TICKETS SOLD

Tour 3 – UNESCO walking tour of Cracow – LIMITED TICKETS
The tour takes place on 29.08 (Tuesday) 15:00-18:00
Walking tour around the Krakow. It includes visiting the old Jewish district of Kazimierz and the Old Town
with the amazing St. Mary’s Church (with the Wit Stwosz Altar) on the Main Square.

160 PLN incl. tax

Beer Club
WHEN? 29.08 (Tuesday) – start at 19:00
WHERE? Stara Zajezdnia Kraków by DeSilva, Świętego Wawrzyńca Street 12, 31-060 Kraków
Get to know Krakow by night - visit one of Krakows’ most popular places for hanging out. As part of the
Beer Club, participants will receive a coupon to use at the venue for a drink.

Tour for the Accompanying person
WHEN? 30.08 (Wednesday) – start st 11:00.
WHERE? Meeting point: Westerplatte Street 20, “Poczta Główna”.
This tour is included in the Accompanying person fee.
A tour created for those who want to learn about the history of the Wawel Castle. During the tour, par-
ticipants will have the opportunity to look into the chambers of the castle, learn many interesting stories
related to them, but also take an unforgettable stroll through the Planty Park, with some non-obvious
stops. Tour includes lunch.
Conference Dinner

WHEN? 31.08 (Thursday) – 18:00 (gathering at 17:30)

WHERE? The buses will pick up the participants from Gronostajowa Street 2, Conference Venue

The return busses will stop at:
1. Conference venue – Gronostajowa street 2
2. Ice krakow – Marii Konopnickiej street 17
3. Old town – Pawia street

The Wieliczka Salt Mine is one of the oldest enterprises in Europe. It has supplied salt to the tables of almost the whole Europe.

Nowadays, it is one of the most frequently visited places in Poland, where intensive conservation works are carried out in order to protect historical sites. With its vast material culture heritage and wealth of inanimate nature, the Wieliczka underground mine is a unique monument on a global scale.

Today, the mine is still an active mining facility, with unique culture, art and traditions dating back many centuries.

The Wieliczka Salt Mine is a monument with centuries of history and cultural heritage, whose rank is emphasised by its presence on the First UNESCO World Cultural and Natural Heritage List. The unique work of nature touched by the hand of man creates a harmonious whole and attracts like a magnet for tourists wishing to discover the mysteries hidden underground. The mine is also an original venue for banquets and concerts.

The underground banquet halls amaze with natural scenery not seen anywhere else. The salt walls shining in shades of grey and silver in the light of crystal chandeliers are very impressive. The conference dinner will take place more than 100 metres below ground. We assure you that you will be enchanted by this venue.

Price: 658 PLN incl. tax
Il Program
Conference Topics

(A) advanced characterization of organic, inorganic, hybrid, and low-dimensional materials
(B) structure and dynamics of molecules
(C) spectroscopy in local fields
(D) vibrational spectroscopy of surfaces and interfaces
(E) nonlinear vibrational spectroscopies
(F) advances in instrumentation
(G) analytical applications to forensics, PAT, works of art, and similar
(H) biodiagnostic spectroscopy
(I) chemometrics and machine learning
(J) computational approaches

Systematic of Presentation Numbers

The type of session and oral presentations (invited/regular) is encoded in the paper numbers as follows: The first letter indicates the session topic of the presentation (A, B, C, etc.), and the last two signs define the type of presentation: P – plenary talk, I – invited talk, O – regular talk, and the number of the talk in particular topic. At ICAVS12 Poster Session 1 (topics: B, C, D) will take place on Monday, August 28, Poster Session 2 (topics: A, E, F, J) on Tuesday, August 29, and Poster Session 3 (topics G, H, I) on Wednesday, August 30. Each poster number includes the letter of the respective topic session. The poster boards are ordered by increasing the poster number.

Oral Presentations

Speakers will be required to report to the technical support staff in the lecture hall of their respective sessions at least 15 minutes prior to the start of the session. Computers running Windows 10 and equipped with both Microsoft Office PowerPoint and Adobe PDF Reader will be provided for presentations in each lecture hall. Please give your presentation on a USB flash drive to the person in charge, who will upload it to the presentation PC and have it ready at the start of your presentation. The presentations will be deleted from the computers after each session.

All lecture halls are equipped with:

- Windows-operating PCs
- LCD projector with single-screen projection configured for 4:3 display aspect ratio
- Wireless remote presenter and laser pointer
- Wireless lavalier microphone
- Speaker timer

Length of oral presentations:

Perspective and plenary lectures: 25 min (+5 min. discussion)
Invited talks: 15 min (+3 min. discussion)
Regular talks: 10 min (+3 min discussion)

As there will be four to five sessions in parallel, we kindly ask you to strictly keep the time.
Poster Presentations
Poster sessions are scheduled from 16:30–18:45 on Monday, 13:15–14:30 on Tuesday, and 16:30–18:45 on Wednesday. Each poster session will be started with flash presentations in room A0-01.

The posters should be put up in the morning of the respective poster session and have to be removed immediately after the poster session finishes.

Please mount your poster on the board with your assigned poster number, e.g. A.18. Posters have to be mounted to poster boards using adhesive tape, which will be provided.

Flash Presentations
Poster flash talks are meant to be a very short (1 minute, only 1 slide) presentation of posters. The author will focus only on the main aim of the research and only mention the key findings. The purpose of the flash talk is to stimulate the audience to view the poster and to discuss the research during the poster session.

A list of all participants who have accepted an invitation for a flash presentation is presented on page 39. The best poster and flash presentations will be rewarded with cash prizes.

Tips For Session Chairs
Arrive at the lecture room of the session at least 10 minutes prior to the start of the session. Confirm the attendance of each presenter and familiarize yourself with the venue and equipment. Check the technology and alert any of the technicians or student volunteers of any problems. Ensure that each presenter has copied their presentation to the presentation computer.

Make sure that the session runs smoothly and on time. Facilitate Q&A and discussion. Keep strictly to the time guidelines to allow for audience participation and to allow audience members to move between sessions. Before the session, remind the speakers of their time limit and agree with them on time signals. A visual cue is less disruptive to the audience than a verbal cue. Use time-keeping signs beforehand.
Kathleen M. Gough
University of Manitoba, Canada

Title of lecture: Progress in infrared spectroscopy

Dr. Kathleen M. Gough is a Professor in the Department of Chemistry, Adjunct Professor in the Department of Physiology and Pathophysiology, and a Core Member of the Biomedical Engineering Graduate Program at the University of Manitoba. She is an expert in vibrational spectroscopy using Far-Field and Near-Field Infrared and Raman microscopes. Her group has been at the forefront of bioapplication developments with the major technological advances in the last decade, including high magnification IR imaging with Focal Plane Array with the original, synchrotron source instrument (IRENI, SRC, Madison WI) and with commercial thermal source IR microscopes, near field IR at the Advanced Light Source (LBL, Berkeley CA) and Optical-Photothermal IR. Her research interests range from biomaterials (cells and nuclei, collagen in tendon and scar, brain and heart tissue, arctic sea ice diatoms, fungi and yeasts) to novel materials (synthetic collagen scaffolds, plant proteins, graphene derivatives). She is an expert in the use of polarized IR to study orientation in collagenous materials. Most recently, she has been collaborating on multi-modal spectroscopy of cells and tissues, sequentially employing far field IR (with Focal Plane Array and with O-PTIR), near field IR with sSNOM, and superresolution fluorescence on the same targets. She is the author of over 100 papers and several book chapters. In 2017, she was elected a Fellow of the Society of Applied Spectroscopy. She serves on the editorial advisory board of Applied Spectroscopy and editorial board of Clinical Spectroscopy. She is a founding member of The International Society for Clinical Spectroscopy (CLIRSPEC) and has served as a council member since its inception.

Laurence A. Nafie
Syracuse University, USA

Title of lecture: Frontiers of Advanced Vibrational Spectroscopy: The Molecular Chirality Perspective

Professor Nafie, Emeritus Distinguished Professor at Syracuse University, received his Ph.D. from the University of Oregon in 1973, studying the theory Raman scattering, and from 1973 to 1975 was a postdoctoral associate at the University of Southern California where he confirmed the discovery of vibrational circular dichroism (VCD). In 1975 joined the faculty at Syracuse University and established a research program in VCD and Raman optical activity (ROA). Among his notable achievements were the first measurements of Fourier transform VCD, the first measurements of scattered (SCP) and dual circular polarization (DCP) ROA, nuclear velocity perturbation (NVP) theory of VCD, now a new accurate method for VCD calculations, electron transition current density (TCD) maps, and finally the theory and confirmation of resonance ROA (RROA). In 1996, he co-founded with Dr. Rina Dukor BioTools, Inc. to commercialize VCD and ROA spectroscopy and was co-chair with Rina of ICAVS-3 in Wisconsin, USA. He has won an Alfred P. Sloan Fellowship (1978) the Bomem-Michelson Award (2001), the Pittsburgh Molecular Spectroscopy Award (2014), the Chirality Medal (2019) for lifetime contributions to molecular chirality, and the Raman Lifetime Achievement Award (2022). In 2010 he became Editor-in-Chief of the Journal of Raman Spectroscopy, and in 2011 he published Vibrational Optical Activity: Principles and Applications by John Wiley & Sons. He has over 300 publications and several patents.
Giulietta Smulevich
University of Florence, Italy

Title of lecture: Strategies and perspectives to investigate the heme-enzymatic mechanism by resonance Raman spectroscopy

Giulietta Smulevich is Professor of Physical Chemistry at the University of Florence. She was visiting and Faculty member at the chemistry Department of Princeton (USA), and visiting Professor at Rutgers U. (USA), Concordia U. (Canada), Buenos Aires U. (Argentina), Berlin technical University (Germany). From 2003 to 2008 she held a position of External Professor, at the Department of Life Sciences (section of Biotechnology), Aalborg University (Denmark). Her research interest has been directed toward the elucidation of the structure-function relationships and catalytic mechanism of heme-containing enzymes from different sources, namely humans, animals, plants, and more recently bacteria, in solutions and crystals, using mainly UV-Vis, resonance Raman and micro-resonance Raman spectroscopy techniques at different temperatures. To date, she is the author of more than 230 scientific papers. In 2022 she has been honored with the Eraldo Antonini Lifetime Achievement Award by the International Society of Porphyrins and Phthalocyanines.
Plenary speakers

Javier Aizpurua
Spanish Council for Scientific Research (CSIC), Spain

Title of lecture: Molecular Optomechanics Approach to Surface-Enhanced Raman Scattering

Javier Aizpurua is a Research Professor of the Spanish Council for Scientific Research (CSIC) at the Center for Materials Physics in San Sebastián, Spain, where he leads the “Theory of Nanophotonics Group” (http://cfm.ehu.eus/nanophotonics). Aizpurua has developed theory to understand the interaction of light and nanostructured materials in a variety of field-enhanced spectroscopy and microscopy configurations, such as in SERS, SEIRA, s-SNOM, STM, or STEM. The understanding of the optical response of complex nanosystems has been the main focus of his research, particularly in the field of optical nanoantennas and nanoplasmonics, with special emphasis on the role of quantum effects in nanophotonics.

Rohit Bhargava
University of Illinois at Urbana–Champaign, USA

Title of lecture: Increasing utility of IR imaging by high performance instrumentation and AI

Rohit Bhargava is a professor of Bioengineering and Founding Director of the Cancer Center at Illinois. He has contributed to the development of infrared spectroscopic imaging, including developments in theory, instruments, applications and data analysis methods. Current work in his laboratory focuses on theoretical modeling that can push the limits of speed and quality of infrared spectroscopic imaging as well as its application. In particular, his group recognize and subtype cancer by its underlying molecular characteristics, by advanced chemical imaging and application of modern machine learning, ultimately allowing for better treatment of patients.

Notburga Gierlinger
University of Natural Resources and Life Sciences, Austria

Title of lecture: Raman Imaging of Plant Cells: probing distribution and orientation of molecules

Notburga Gierlinger (Assoc. Prof.) is heading the research group “Biological materials on the nano- and microscale” (www.bionami.at) at the Institute of Biophysics at the University of Natural Resources and Life Sciences (BOKU, Vienna). She has focused on Raman microscopy applications on biological materials since 2 decades with research positions at Max Planck Institute of Colloids and Interfaces (Biomaterials, Potsdam Germany), JKU (Linz, Austria) and ETH (Building Materials, Zürich, Switzerland). Her emphasis is on revealing the chemistry in context with the microstructure of plant tissues to retrieve structure-function relationships. Research projects include plant cell walls, plant surfaces and interfaces and include, various plant organs (stems, root, leaves...) as well as different plant species (algae, arabidopsis, nutshells (ERC consolidator grant), wood...).
Koichi Iwata
Gakushuin University, Japan

Title of lecture: Bimolecular chemical reactions in solution examined with time-resolved infrared and Raman spectroscopy

Koichi Iwata received Dr.Sci. from Department of Chemistry, The University in 1989. He was engaged in spectroscopic studies at The Ohio State University as a postdoctoral fellow, at Kanagawa Academy of Science and Technology (KAST) as a researcher, and Department of Chemistry, The University of Tokyo as an associate professor. He joined Department of Chemistry, Faculty of Science, Gakushuin University as a professor in 2009. He currently serves as the president of the Spectroscopical Society of Japan (SjSJ) and the section editor for theoretical and physical chemistry of Bulletin of the Chemical Society of Japan (BCSJ). His research interests include the development of new spectroscopies and the examination of dynamic processes in complex systems.

Sergei G. Kazarian
Imperial College London, United Kingdom

Title of lecture: Advances in Infrared Spectroscopic Imaging

Sergei G. Kazarian is Professor of Physical Chemistry in the Department of Chemical Engineering at Imperial College London, consistently one of the world’s top ten universities. His scientific research began in Armenia using infrared spectroscopy to study matrix isolation of weak complexes of CO2 with metal atoms. Now, his research encompasses the fields of advanced vibrational spectroscopy, supercritical fluids, intermolecular interactions and materials. In last two decades, his research has mainly been focused on developing and applications of FTIR spectroscopic imaging to materials, biomedical samples and pharmaceuticals, along with tip-enhanced Raman scattering for nanomaterials (www.imperial.ac.uk/vsci). He also contributed to the fields of microfluidics, forensic science and analysis of objects of cultural heritage. Sergei Kazarian has published nearly 300 articles and reviews in leading scientific journals and he is Editor in Chief of Applied Spectroscopy. He was awarded the RSC Sir George Stokes Award for his research with ATR-FTIR spectroscopic imaging in 2015.

Dongho Kim
Yonsei University, Korea

Title of lecture: Ultrafast Structural Dynamics in Various π-Conjugated Molecular Systems Probed by Time-resolved Electronic and Vibrational Spectroscopy

Dongho Kim is a Professor at the Department of Chemistry Yonsei University. His cutting edge research focuses on various dimensions of aromaticity and antiaromaticity in molecular systems. In particular, Professor Kim has received worldwide recognition for his work on Möbius aromaticity. He has published more than 530 article in SCI journals and been cited almost 19,000 times by other scholars. In recognition of the quantity and quality of his research output, Professor Kim was selected as the first National Scholar in 2007, and he received a Presidential Award for his Korean Science Prize in Chemistry. Prof Kim was honoured with numerous awards in recognition of outstanding research accomplishments, including recently: selected as 100 National Research and Development Excellent Achievements Best Achievement in Basic Science & Infrastructure field (Ministry of Science and ICT) (2017), 4th FILA Basic Science Award (The Korean Academy of Science and Technology) (2017), National Medal for the Science and Technology (Ministry of Science and ICT) (2017), Academic Excellence Prize (Korean Chemical Society) (2018), The JPA Honda-Fujishima Award (The Japanese Photochemistry Association) (2019), Hans Fisher Award (Society of Porphyrins & Phthalocyanines) (2020), Sudang Prize (Sudang Foundation) (2020), Toray Prize (Toray Science & Technology Foundation) (2022). Currently, he is an editorial board member of the American Chemical Society’s Journal of Physical Chemistry.
Axel Mosig

Ruhr University Bochum, Germany

Title of lecture: Theory is dead, long live theory: Hypothesis-centric machine learning in vibrational spectroscopy

Axel Mosig is a Professor for Bioinformatics at the Ruhr University Bochum, Germany. Axel was received his undergraduate and graduate education in Computer Science at the University of Bonn, where he received his Dr. rer. nat. degree in 2004. After a postdoc at the University of Leipzig, Germany, where he worked on computational structural biology in 2004-2005, he moved to Shanghai as a postdoctoral researcher and founding member of the CAS-Max Planck Partner Institute for Computational Biology (PICB), where in 2008 he started his own research group as a PI computational approaches for bioimage analysis. In 2011, he joined the Faculty of Biology and Biotechnology at the Ruhr University Bochum, where since 2019 he is also heading the Bioinformatics Department of the Research Center for Protein Diagnostics (PRODI). Axel's research is driven by the overarching quest to understand how computational models relate to and affect the experimental life sciences. His research at PRODI is focused on machine learning for analyzing and understanding patterns of disease in infrared microscopic images.

Alison Rodger

Macquarie University, Australia

Title of lecture: Can attenuated total reflectance infrared spectroscopy (ATR-IR) be used with polarised light?

Alison Rodger is a biophysical chemist who invents and develops spectroscopic methods to characterise the structure and function of biomacromolecules and their assemblies. Her career began with a PhD in Australia then moved to the UK for 30 years before returning to Australia in 2017. She has published over 200 papers, 9 books, 40 book chapters, and 5 patents. She was recognised in the 2015 Analytical Science Power List, is an Honorary Fellow of the British Biophysical Society, a Fellow of the Royal Society of Chemistry where she served as a member of the Council, Fellow of the Royal Australian Chemical Institute, and Fellow of the Australian Academy of Science.

Angela R. Hight Walker

National Institute of Standards and Technology, USA

Title of lecture: In-Operando Magneto-Raman Study of Graphene Device in the Quantum Hall Regime

Dr. Hight Walker is a senior scientist at the National Institute of Standards and Technology (NIST), where she began her career as a National Research Council Postdoctoral Fellow. Her research focuses on advancing optical spectroscopies and their applicability to characterize quantum nanomaterials. Her research team has developed unique hyphenated techniques such as magneto-Raman, where samples are probed as a function of laser wavelength, temperature, magnetic field and back gating. These novel capabilities probe the underlying photophysics of nanomaterials. An issue of great importance to Angela is encouraging the young and under-resourced to participate in science. Through demonstrations and lectures, she actively engages in promoting the excitement of science. Recruiting, supporting, and mentoring students and postdoctoral researchers is a passion. Dr. Hight Walker is presently the Chair of the APS Committee on the Status of Women in Physics (CSWP).
Julia Weinstein

University of Sheffield, United Kingdom

Title of lecture: Towards vibrational control of electron transfer with short IR pulses

Julia Weinstein is a Professor of Physical Chemistry at the University of Sheffield, UK. Julia was educated at Moscow Lomonosov State University, Russia (PhD in electron transfer, 1994, under supervision of Prof M Kuzmin and Prof N Sadovskii). After PhD, she became a member of academic staff, working on photochemistry of coordination compounds. In 2000 – 2004, she joined the University of Nottingham, UK, first as a Royal Society/NATO Postdoctoral Fellow, and then as a temporary lecturer (Assistant Professor). In 2004, Julia was awarded a 5-year EPSRC Advanced Research Fellowship to work on light-driven processes in metal chromophores. She moved to the University of Sheffield in 2005, where she is currently Professor of Physical Chemistry. Julia’s interests are in ultrafast electronic, structural, and spin dynamics of molecules and materials. She leads the Lord Porter Laser Laboratory in Sheffield, which comprises a combination of electronic and vibrational spectroscopies, including time-resolved infrared and 2DIR spectroscopies, and ultrafast fluorescence upconversion. Recent scientific developments include multipulse experiments to control excited state dynamics, and application of ultrafast X-ray sources at XFELs to “watch chemistry happen”. Julia’s long term collaborations include Laser for Science Facility in the UK, and multiple research groups in the UK and abroad. She is a recipient of the 2017 RSC Chemical Dynamics Award.
Invited speakers

(A) advanced characterization of organic, inorganic, hybrid, and low-dimensional materials

Marco Daturi
Universite de Caen Normandie
France

Christiane Höppener
University of Jena
Germany

Joanna Profic-Paczkowska
Jagiellonian University
Poland

Marek Procházka
Charles University
Czech Republic

(B) structure and dynamics of molecules

Petra Hellwig
University of Strasbourg
France

Piotr Mak
Saint Louis University
USA

Barbara Rossi
Elettra Sincrotrone Trieste
Italy

Jianping Wang
Chinese Academy of Sciences
China

Lauren Webb
The University of Texas at Austin
USA

Tobias Weidner
Aarhus University
Denmark

(C) spectroscopy in local fields

Jeremy Baumberg
University of Cambridge
UK
(D) vibrational spectroscopy of surfaces and interfaces

Patrycja Kielb
University of Bonn
Germany

Jacek Kozuch
Freie Universität Berlin
Germany

Hoang Khoa Ly
Technische Universität Dresden
Germany

Judith Langer
CIC biomaGUNE
San Sebastián
Spain

Bin Ren
Xiamen University
China
(E) nonlinear vibrational spectroscopies

Julianne Gibbs-Davis  
University of Alberta  
Canada

Zsuzsanna Heiner  
Humboldt Universitat zu Berlin  
Germany

Kotaro Hiramatsu  
The University of Tokio  
Japan

Satoshi Nihonyanagi  
RIKEN  
Japan

Kailash Chandra Jena  
Indian Institute of Technology Ropar  
India

Dennis Hore  
University of Victoria  
Canada

(F) advances in instrumentation

Krzysztof Banaś  
National University of Singapure  
Singapore

Ariane Deniset-Besseau  
Université Paris-Saclay  
France

Kishan Dholakia  
University of St Andrews  
UK

Torsten Frosch  
Technische Universität Darmstadt  
Germany

Bernhard Lendl  
Technische Universität Wien  
Austria

Kerstin Ramser  
Lulea University of Technology  
Sweden
(G) analytical applications to forensics, PAT, works of art, and similar

Entesar Al-Hetlani  
Kuwait University  
Kuwait

Keith Gordon  
Otago University  
New Zealand

Agnieszka Kamińska  
Polish Academy of Sciences  
Poland

Maria Paula Marques  
University of Coimbra  
Portugal

Lisa Vaccari  
Elettra-Sincrotrone Trieste  
Italy

Bayden Wood  
Monash University  
Australia

(H) biomedical/biodiagnostic spectroscopy

Claude Aguergaray  
University of Auckland  
New Zealand

Jaebum Choo  
Chung-Ang University  
South Korea

Beata Brozek-Pluska  
Technical University of Lodz  
Poland

Renzo Vanna  
IFN – CNR & Politecnico di Milano  
Italy

Cristina Zavaleta  
University of Southern California  
USA
Ben Gardner
University of Exeter
UK

Fay Nicolson
Dana Farber Cancer Institute
USA

Hidetoshi Sato
Kwansei Gakuin University
Japan

(I) chemometrics and machine learning

David Pérez Guaita
University of Valencia
Spain

Bogumila Kupcewicz
Nicolaus Copernicus University in Torun
Poland

Valeria Tafintseva
Norwegian University of Life Sciences
Norway

(J) computational approaches

Petr Bouř
Czech Academy of Science
Czech Republic

Joanna Rode
Institute of Nuclear Chemistry and Technology
Poland
Flash Presentations

Session A

Yiqing Feng
Investigating NBD-CI and its derivative NBD-Ceramide in living cells using surface enhanced Raman scattering

Tetiana Stepanenko
Molecular Profiling of Erythrocyte Membrane at the Nano-Scale and at the Single Molecule Level

Hadass Tischler
Super-Resolution Raman Spectroscopy—Applications to Diamond Identification

Martina Zangari
FTIR microscopy and nanoscopy analysis of protein-fiber interaction in asbestos body model assembling

Session B

Maxim Bokov
Rearrangement of intracellular crystalline guanine as an adaptation for various illumination levels

Agnieszka Domagała
Protein structure investigation via ROA-CPL spectroscopy and Eu(III) probe

Andrea Dali
Spectroscopic characterization of the coproporphyrin ferrochelatase from Corynebacterium diphtheriae

Monika Hałat
Raman Optical Activity is a sensitive tool to detect changes in the structure of biomolecules and supramolecules

Štěpán Jílek
Formation and Behavior of Guanosine-5’-Monophosphate assemblies at low pH: temperature and cation effects

Chara Karafoulidi-Retsou
Characterizing the large subunit of a membrane-bound [NiFe] hydrogenase by combined IR spectroscopic and computational studies

Petra Maleš
The revelation of interactions in model myelin with FTIR spectroscopy

Fatima Matroodi
Spectral features of Interfacial Water in Imidazolium-based Ionic Liquids/water mixtures: UV Resonance Raman Approach

Katarzyna Pajor
How to properly register Raman optical activity spectra of chiral and light-absorbing biomolecules?

Sung Man Park
Conformational study by IR resonant VUV-MATI mass spectroscopy

Patryk Pyrcz
Temporal Evolution of Single-Molecule Surface-Enhanced Raman Scattering Spectra

Naoki Sakurai
Conformation of choline-chloride-based deep eutectic solvents and its temperature dependence observed with Raman spectroscopy

Věra Schrenková
Characterization of sofosbuvir polymorphs using polarized Raman microscopy

Cecilia Spedalieri
UV resonance Raman of serum albumins

Risa Suzuki
Formation of vitamin D3 observed by picosecond time-resolved Raman spectroscopy

Session C

Cherine Alaouta
Development of high-Throughput Raman imaging to investigate the efficacy of Doxifluridine Squalenoyl nanomedicine on single breast cancer cells

Shrobona Banerjee
Surface-enhanced Raman scattering (SERS) of biomolecules – Can the variations tell a story?
Ioana Marica  Optical properties and SERS analysis of quasi-3D plasmonic nanostructures fabricated by colloidal lithography

Beata Wrzosek  A new approach in the SERS blinking analysis

**Session D**

Ilirjana Bajama  Dual-tag paradigm in SERS analysis for removal of antibiotics and dyes from waste water treated with biogenic carbonate powder nanoparticles

Yi-Fan Bao  AFM-based non-gap mode tip-enhanced Raman spectroscopy (TERS)

Amanda Bartkowiak  Application of Resonance Raman Spectroscopy for label-free differentiation of ferrous and ferric cytochrome c

Lars Dannenberg  Monitoring plasmon-mediated chemical reactions on immobilized noble metal nanoparticles

Paul Kerner  Atomic-scale dynamics in plasmonic hotspots: fast SERS of picocavities

Adrian Warzybok  Photo-induced enhanced Raman spectroscopy on thin Ag-TiO2 nanoplatforms: a study of mechanisms and influence of visible light

Li Zhang  Understanding Structure, Interference, and Absorption effects in Vibrational SFS Experiments

**Session E**

Aruna Kumarasiri  Electronic Structure of para-Cyanophenol at the Air-Aqueous Interface from Vibrational Sum Frequency Generation Spectroscopy

**Session F**

Shiwani  High-Throughput Raman System for Rapid Microplastic Characterization

**Session G**

Meshari Al-Qalfas  Assessment of the effects of Kuwait’s high temperatures and humidity on whole blood stains stability on fabric using ATR-FTIR spectroscopy

Loren Christie  Cell metabolite quantification using the Dxcover infrared platform

Víctor Navarro Esteve  Poc quantification and profiling of urine cells by integrating cytocentrifugation and ir mesurements on the same substrate

Felix Frank  A new sensitive multi-analyte VOC sensor based on an integrated optics waveguide coated with a functionalised mesoporous sensing layer and QCL-IR spectrometry

Jiro Karlo  Exploring potential of reverse Raman Stable Isotope Probing and 2D correlation spectroscopy in monitoring metabolic pathway dynamics in situ.

Alžbeta Kuižová  Drop coating deposition Raman spectroscopy (DCDRS) as a tool for rapid determination and identification of contaminants and food additives

Marika Niihori  Towards the intelligent toilet: SERS sensing of nM-level neurotransmitters with Fe-sensitized self-assembled gold nanoparticle arrays

Shravan Raghunathan  Bio-chemical assessment of blood cell and PBMC smears using optical photothermal mid-IR spectroscopy for studies of diseases and infections

Gohar Soufi  Identification and classification of methotrexate and its metabolites in human serum samples using surface-enhanced Raman scattering combined with advanced data analysis
Chiaramaria Stani  
FTIR nano-spectroscopy at SISSI-Bio Beamline: recent insight in the field of Cultural Heritage

Session H

Masoumeh Alinaghi  
Strong impact of de novo purine biosynthesis on the spectroscopic signature of Staphylococcus aureus revealed by the screening of a gene-defined transposon mutant library

Helena Friedrich  
Metabolic impacts of microplastic exposure in mammalian cells measured via FTIR microspectroscopy

Wiktoria Korona  
Non-label identification of acute myeloid leukemia with FLT3 gene mutation using Raman spectroscopy

Mateusz Mignalski  
Raman and Resonance Raman Spectroscopy for Malaria Red Blood Cells Analysis

Muhammad  
SERS-imaging for probing program death ligand-1 immunomarker in real-time tumour progression

Aleksandra Pragnąca  
Spectroscopic detection of hypoxic state in the brain endothelium and endothelial progenitor cells

Ota Samek  
Effects of antimicrobials on microbial Raman spectra as the first step for detection of antimicrobial resistance

Kacper Siąkała  
Spectroscopic analysis of the fatty acids uptake by human leukemic cells and accompanying metabolic changes

Kacper Stawowski  
Differentiation and classification of leukemic cells with the use of Raman Imaging

Jizhou Zhong  
Discovery of novel spectral biomarkers for early diagnosis of Lyme Disease

Session I

Tarek Eissa  
In silico modeling reveals the prospects and limitations of vibrational fingerprinting for phenotyping biological systems

Jaume Béjar Grimalt  
Monitoring of physical effort by infrared spectroscopy of urine composition

Azadeh Mokari  
Pre-processing Raman data via deep learning method

Session J

Julian Mateo Rayo Alape  
Vibrational calculations and SERS activity prevision of hepcidin hormone: contribution for hyperinflammation screening

Corentin Grassin  
IR/VCD spectroscopic studies on matrix-isolated chiral 1-phenyl-1-propanol

Jana Hudecová  
Structure of Histidine-Metal Complexes in Solution Revealed by Raman Optical Activity

Mohammed Siddhique  
Development of Computational Models to Decipher Raman Optical Activity Spectra of G-quadruplexes

Para Kkadan  
Optical Activity Spectra of G-quadruplexes
Program

11:00-12:00 Registration
11:30-13:30 Workshop Session
12:00-13:00 Workshop session 1 [Parallel ROOM A0-01]
15:00-17:00 Workshop session 2 [Parallel ROOM A0-02, Parallel ROOM A0-04]
17:00-18:00 Coffee break
17:30-19:00 Perspectives Session ROOM A0-01 (Chair: Einar Baldursson, Magni Magnússon, Kaustuv Roy, Haraldur Ólafsson)
18:00-20:30 Program: Social events, scheduled in the pigeon house complex
19:00-20:30 Welcome Cocktail - Conference Welcome

8:45-9:00 Opening Ceremony [Meeting Room ROOM A0-01]
Opening Remarks (Chair: Gudleikur Gudmundsdottir)...
9:00-9:15 Opening Ceremony [Meeting Room ROOM A0-01]
Opening Remarks (Chair: Gudleikur Gudmundsdottir)...
9:15-9:45 Opening Ceremony [Meeting Room ROOM A0-01]
Opening Remarks (Chair: Gudleikur Gudmundsdottir)...

Thursday

10:15-10:45 Coffee Break
10:45-12:00 Plenary Session 1 (Chair: Valery A. Konstantinov, Toshiyuki Yamasaki)
10:45-12:00 Plenary Session 1 (Chair: Valery A. Konstantinov, Toshiyuki Yamasaki)
10:45-12:00 Plenary Session 1 (Chair: Valery A. Konstantinov, Toshiyuki Yamasaki)
10:45-12:00 Plenary Session 1 (Chair: Valery A. Konstantinov, Toshiyuki Yamasaki)

Friday

14:30-15:00 Coffee Break
14:00-15:00 Plenary Session 1 (Chair: Gudleikur Gudmundsdottir)...
14:00-15:00 Plenary Session 1 (Chair: Gudleikur Gudmundsdottir)...
14:00-15:00 Plenary Session 1 (Chair: Gudleikur Gudmundsdottir)...
14:00-15:00 Plenary Session 1 (Chair: Gudleikur Gudmundsdottir)...

Saturday

11:00-12:30 Lunch
18:00-20:30 Closing Ceremony [Meeting Room ROOM A0-01]
## Thursday

### 10:45-12:10

**SESSION 1**

<table>
<thead>
<tr>
<th>Chair: Aga Prystowska</th>
<th>Chair: Ursula Heinen</th>
<th>Chair: Alexander Stepanov</th>
<th>Chair: Michael Müller</th>
</tr>
</thead>
<tbody>
<tr>
<td>10:55-10:55 R. Sen</td>
<td>11:00-11:05 S. K. D. Kuruvilla</td>
<td>11:00-11:05 S. Hirose</td>
<td>11:05-11:10 H. Tanaka</td>
</tr>
</tbody>
</table>

### 12:10-13:40

**Lunch**

### 13:40-15:00

**SESSION 2**

<table>
<thead>
<tr>
<th>Chair: Maksim Ostroumov</th>
<th>Chair: James Ostroumov</th>
<th>Chair: Ali R. Sattar</th>
<th>Chair: Ji-han Lee</th>
</tr>
</thead>
<tbody>
<tr>
<td>13:55-14:10 T. Maeda</td>
<td>14:00-14:05 Y. Matsuura</td>
<td>14:05-14:10 S. Mimura</td>
<td>14:10-14:15 H. Mimura</td>
</tr>
<tr>
<td>14:25-14:30 C. Mihalik</td>
<td>14:30-14:35 Y. Watanabe</td>
<td>14:35-14:40 S. Kusunoki</td>
<td>14:40-14:45 R. Gourley</td>
</tr>
</tbody>
</table>

### 15:00-16:20

**SEMM POL presentation ROOM A0-01**

### 16:20-18:00

**Conference Dinner**

## Friday

### 10:15-11:45

**SESSION 1**

<table>
<thead>
<tr>
<th>Chair: Milu Prystowska</th>
<th>Chair: Thomas Heinen</th>
<th>Chair: Sagie Katz</th>
<th>Chair: Benjamin Proof</th>
</tr>
</thead>
</table>

### 12:00-12:30

**SEMM POL presentation ROOM A0-01**

### 12:30-13:00

**Club Awards**

### 13:00-13:30

**Lunch**

### 13:45-15:15

**Award & Closing Ceremony ROO A0-01**

### 15:15-16:45

**Summary of SEMS 12 and Good Bye**

---

**Friday:**

- **10:15-11:45:** SESSION 1
- **12:00-12:30:** Club Awards
- **13:00-13:30:** Lunch
- **13:45-15:15:** Award & Closing Ceremony

---

**Thursday:**

- **10:45-12:10:** SESSION 1
- **12:10-13:40:** Lunch
- **13:40-15:00:** SEMM POL presentation
- **16:20-18:00:** Conference Dinner
# Detailed program

## Sunday

<table>
<thead>
<tr>
<th>Time</th>
<th>Location</th>
<th>Event</th>
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</thead>
<tbody>
<tr>
<td>11:00-20:00</td>
<td>Room</td>
<td>Registration</td>
</tr>
<tr>
<td>11:30-17:15</td>
<td>Workshop</td>
<td>Workshop Session</td>
</tr>
<tr>
<td>11:30-13:30</td>
<td>A0-01</td>
<td>Workshop session 1 HORIBA/COMEF Raman imaging: discover the easiest and the most accurate ways to characterize micro &amp; nano-plastics. Combine its full power to all your microscope in your lab with correlative microscopy.</td>
</tr>
<tr>
<td>13:30-15:30</td>
<td>A0-03</td>
<td>Workshop session 2 WiTec Raman Workshop New Perspectives in 3D Raman Imaging and Correlative Techniques</td>
</tr>
<tr>
<td>13:30-15:30</td>
<td>A0-04</td>
<td>Workshop session 2 Photothermal: O-PTIR Workshop Submicron IR and Simultaneous Raman Microscopy with Co-Located Fluorescence Imaging</td>
</tr>
<tr>
<td>15:30-17:15</td>
<td>A0-01</td>
<td>CLIRSPEC session</td>
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<tr>
<td>17:00-17:30</td>
<td></td>
<td>Coffee break</td>
</tr>
<tr>
<td>17:30-19:30</td>
<td>A0-01</td>
<td>Perspective Session Chairs: Kamilla Malek, Małgorzata Baranska, Janina Kneipp, Katarzyna Majzner</td>
</tr>
<tr>
<td>17:30-17:55</td>
<td>A0-01</td>
<td>Progress in infrared spectroscopy Kathleen Gough¹&lt;br&gt;¹University of Manitoba</td>
</tr>
<tr>
<td>18:05-18:30</td>
<td>A0-01</td>
<td>Frontiers of Advanced Vibrational Spectroscopy: The Molecular Chirality Perspective Laurence Naife¹&lt;br&gt;¹Syracuse University</td>
</tr>
<tr>
<td>18:40-19:05</td>
<td>A0-01</td>
<td>Strategies and perspectives to investigate the heme-enzymatic mechanism by resonance Raman spectroscopy Giulietta Smulevich¹&lt;br&gt;¹Dipartimento di Chimica “Ugo Schiff” (DICUS), Università di Firenze</td>
</tr>
<tr>
<td>19:30-21:30</td>
<td></td>
<td>Welcome Cocktail – Conference Venue</td>
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<tr>
<td>21:00-23:00</td>
<td></td>
<td>Dinner</td>
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## Monday

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<thead>
<tr>
<th>Time</th>
<th>Location</th>
<th>Event</th>
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</thead>
<tbody>
<tr>
<td>9:00-10:15</td>
<td>A0-01</td>
<td>Plenary Session Chairs: Bin Ren, Harumi Sato</td>
</tr>
<tr>
<td>9:00-9:30</td>
<td>A0-01</td>
<td>Can attenuated total reflectance infra red spectroscopy (ATR-IR) be used with polarised light? Alison Rodger¹, Paul Wormell², Jun Koshubu³, Junya Kitamura³, Akihiro Sato³&lt;br&gt;¹Macquarie University</td>
</tr>
<tr>
<td>10:15-10:45</td>
<td></td>
<td>Coffee Break</td>
</tr>
<tr>
<td>10:45-12:10</td>
<td>A0-01</td>
<td>SESSION 1</td>
</tr>
<tr>
<td>10:45-11:00</td>
<td>A1-01</td>
<td>(B) Structure &amp; dynamics of molecules Chair: Ewan Blanch</td>
</tr>
<tr>
<td>10:45-11:00</td>
<td>A0-01</td>
<td>Probing the active site structural changes in P450/P420 forms of CYP121 Piotr Mak¹&lt;br&gt;¹Saint Louis University</td>
</tr>
<tr>
<td>11:05-11:20</td>
<td></td>
<td>Insights into molecules structure and dynamics by multi-wavelengths UV Resonance Raman spectroscopy Barbara Rossi¹&lt;br&gt;¹Elettra Sincrotrone Trieste</td>
</tr>
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<td>Time</td>
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<td>Authors</td>
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<tr>
<td>11:25-11:35</td>
<td>Detection, characterization, and differentiation of SHb and HbFeIII–SH adducts inside functional erythrocytes</td>
<td>Jakub Dybaś¹, Tetiana Stepanenko², Grzegorz Zajac¹, Katarzyna M. Marzec³</td>
</tr>
<tr>
<td>11:40-11:50</td>
<td>Revealing the problem of the effective charge of iron ion in oxy-haemoglobin molecule</td>
<td>Katarzyna Dziedzic-Kocurek¹, Jakub Dybaś², Jan Stanek¹</td>
</tr>
<tr>
<td>11:55-12:05</td>
<td>Understanding Hydrogenases by 2D-IR Spectroscopy and Vibrational Perturbation Theory</td>
<td>Marius Horch¹, Yvonne Rippers¹, Cornelius Bernitzky¹, Solomon Wrathall², Barbara Procacci², Janna Schöcknecht³, Claudia Schulz³, Christian Lorent³, Catharina Kulk-Peschke³, James Birrell⁴, Ingo Zebger⁵, Gregory Greetham⁵, Oliver Lenz⁵, Neil Hunt²</td>
</tr>
</tbody>
</table>

**A1-02 (C) Spectroscopy in local fields**
Chair: Volker Deckert

<table>
<thead>
<tr>
<th>Time</th>
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<th>Authors</th>
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</thead>
<tbody>
<tr>
<td>10:45-11:00</td>
<td>Probing protein conformations at the nanoscale by means of IR nanospectroscopy</td>
<td>Antonia Intze¹, Maria Eleonora Temperini², Raffaella Polito², Michele Ortolani², Valeria Giliberti³</td>
<td>Istituto Italiano di Tecnologia, Center for Life Nano- and Neuro-Science¹, Department of Physics, Sapienza University of Rome², Istituto Italiano di Tecnologia, Center for Life Nano- and Neuro-Science³</td>
</tr>
<tr>
<td>11:05-11:20</td>
<td>Nanophotonic platforms for enhanced chirally sensitive vibrational spectroscopy</td>
<td>Malcolm Kadodwala¹</td>
<td>University of Glasgow¹</td>
</tr>
<tr>
<td>11:25-11:35</td>
<td>Viewing interfacial chemistry through a graphene window with broadband infrared nanospectroscopy</td>
<td>Hans Bechtel¹, Jonathan Larson², Xiao Zhao², Xin He², Dong Li², Behzad Rad², Chunsheng Yan², Paul Ashby³, Stephanie Gilbert Corder³, Robert Kostecki³, Miquel Salmeron³</td>
<td>Advanced Light Source, Lawrence Berkeley National Laboratory³, Energy Storage &amp; Distributed Resources Division, Lawrence Berkeley National Laboratory³, Materials Sciences Division, Lawrence Berkeley National Laboratory³, Molecular Foundry, Lawrence Berkeley National Laboratory³</td>
</tr>
<tr>
<td>11:40-11:50</td>
<td>Comparison of resonant and non-resonant reporter for the selection of brightest gold nanoparticles for Surface-enhanced Raman spectroscopy.</td>
<td>Megha Mehta¹, William Skinner¹, Sara Mosca², Benjamin Gardner¹, Francesca Palombo¹, Pavel Matousek², Nicholas Stone¹</td>
<td>University of Exeter¹, STFC Rutherford Appleton Laboratory²</td>
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</tbody>
</table>

**A0-04 (F) Advances in instrumentation**
Chair: Kerstin Ramser

<table>
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<th>Time</th>
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<th>Authors</th>
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<tr>
<td>10:45-11:00</td>
<td>Comparison of ATR-FTIR and O-PTIR techniques at ISMI beamline for the characterisation of biological and cultural heritage samples</td>
<td>Krzysztof Banas¹, Agnieszka Banas¹, Mark Breese¹</td>
<td>Singapore Synchrotron Light Source¹</td>
</tr>
<tr>
<td>11:05-11:20</td>
<td>Emerging Trend in AFM-IR: Surface-sensitive mode to probe sample's very surface</td>
<td>Ariane Deniset-Besseau¹, Jérémie Mathurin², Alexandre Dazzi²</td>
<td>Institut de Chimie-Physique, Université Paris-Saclay¹, Institut de Chimie-Physique, CNRS²</td>
</tr>
</tbody>
</table>
SR-FTIR Imaging of Live Cells Using a Novel Demountable Flow System to Study Phospholipidosis
Ohood Alshareef1, K.L Andrew Chan1, Ben Forbes1, Mohamed Alhnan1, Gianfelice Cinque2
1Institute of Pharmaceutical Sciences, King's College London
2Diamond Light Source, Harwell Science and Innovation Campus

Infrared spectroscopy at the user facility ELI Beamlines
Nils Lenngren1, Mateusz Rebarz1, Jakob Andreasson1, Miroslav Kloz1
1The Extreme Light Infrastructure ERIC

Current status of Chemical Infrared Imaging (CIRI / SOLAIR) beamline in Solaris
Maciej Roman1, Danuta Liberda1, Paulina Koziol1, Karolina Kosowska1, Tomasz P. Wrobel1
1SOLARIS National Synchrotron Radiation Centre, Jagiellonian University

SERS combined with chemometric analysis for detection and identification of microorganisms: viruses and bacteria.
Agnieszka Kamińska1, Krzysztof Niciński1, Sylwia Berus1, Dorota Korsak2, Tomasz Szymborski1, Beata Młynarczyk-Bonikowska1, Monika Adamczyk-Popławska2, Evelin Witkowska1
1Institute of Physical Chemistry, Polish Academy of Sciences
2University of Warsaw, Faculty of Biology, Institute of Microbiology

SISSI-Bio: the multipurpose infrared laboratory at Elettra synchrotron facility
Lisa Vaccari1, Giovanni Birarda1, Frederica Piccirilli1, Diana Eva Bedolla2, Chiaramaria Stani3
1Elettra Sincrotrotrone Trieste
2Area Science Park
3CERIC-ERIC

Electrostatic and electrodynamic fields in lipid bilayer membranes
Lauren Webb1
1The University of Texas at Austin

Probing protein structure on nanoparticle surfaces using theoretical and experimental sum frequency scattering spectroscopy
Tobias Weidner1
1Department of Chemistry, Aarhus University, Denmark, email: weidner@chem.au.dk

FTIR studies of mutual interaction in PLL-doped DPPC/DPPG membranes: a powerful insight by chemometric analysis
Paulina Trombik1, Miroslaw Czarnecki1, Katarzyna Cieślińska-Boczula1
1Faculty of Chemistry, University of Wroclaw, F. Joliot-Curie 14, 50-383 Wroclaw

Crystalline purines in microalgae: Surprising robustness of the biosynthesis of crystalline guanine in dinoflagellates
Peter Možes1, Maxim Bokov1, Radek Bura1, Jana Pilátová2
1Charles University, Faculty of Mathematics and Physics, Institute of Physics
2Charles University, Faculty of Science, Department of Experimental Plant Biology
<table>
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<tr>
<th>Time</th>
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<th>Affiliations</th>
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<tr>
<td>13:10-13:25</td>
<td><strong>Surface-Enhanced Anti-Stokes Intensity Fluctuations at High Speed</strong></td>
<td>Alexandre Brolo¹, Nathan Lindquist²</td>
<td>¹University of Victoria, ²Bethel University</td>
</tr>
<tr>
<td>13:30-13:45</td>
<td><strong>Spectrally Resolved Super-Resolution Surface Enhanced Raman Scattering Imaging</strong></td>
<td>Zachary Schultz¹</td>
<td>¹The Ohio State University</td>
</tr>
<tr>
<td>13:50-14:00</td>
<td><strong>Beyond the metal core: leveraging stabilizer-metal interactions for direct SERS detection</strong></td>
<td>Chiara Deriu¹, Laura Fabris¹, Politecnico di Torino</td>
<td></td>
</tr>
<tr>
<td>14:05-14:15</td>
<td><strong>Exploring and Optimizing Factors Influencing Surface-Enhanced Raman Scattering (SERS) Performance</strong></td>
<td>Sylvester Gawinkowski¹</td>
<td>¹Institute of Physical Chemistry, Polish Academy of Sciences</td>
</tr>
<tr>
<td>14:20-14:30</td>
<td><strong>In vivo Real-time Multiplex Detection of Plant Signalling Molecules Using Surface-Enhanced Raman Scattering Nanosensor</strong></td>
<td>Won Ki Son¹</td>
<td>¹Seoul National University</td>
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<tr>
<td></td>
<td><strong>F</strong> Advances in instrumentation</td>
<td>Chair: Agnieszka Banas</td>
<td></td>
</tr>
<tr>
<td>13:10-13:20</td>
<td><strong>Dxcover® Platform: The next generation of ATR-FTIR spectroscopy</strong></td>
<td>Holly Butler¹, Loren Christie¹, Matthew J. Baker²</td>
<td>¹Dxcover Ltd, ²School of Medicine, University of Central Lancashire</td>
</tr>
<tr>
<td>13:25-13:35</td>
<td><strong>Infrared nanoimaging and nanospectroscopy – emerging tools for physical and (bio)chemical nanoanalytics</strong></td>
<td>Adrian Cernescu¹</td>
<td>¹attocube systems AG</td>
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<tr>
<td>13:40-13:50</td>
<td><strong>Most recent advances of QCL-IR microspectroscopy</strong></td>
<td>Matthias Godejohann¹</td>
<td>¹MG Optical Solutions</td>
</tr>
<tr>
<td>13:55-14:05</td>
<td><strong>Widefield Super-Resolution IR Imaging with Fluorescence Enhanced Photothermal Infrared</strong></td>
<td>Miriam Unger¹, Mustafa Kansiz¹</td>
<td>¹Photothermal Spectroscopy Corp</td>
</tr>
<tr>
<td>14:10-14:20</td>
<td><strong>Nano-Sized and Wearable Raman Spectrometers: Towards Widespread of SERs and Vibrational Spectroscopy</strong></td>
<td>William Terziyan¹, Daniel Lauriola¹, Chase Wang¹</td>
<td>¹BaySpec, Inc.</td>
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<td><strong>G</strong> Analytical applications</td>
<td>Chair: Yaakov Tischler</td>
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<tr>
<td>13:10-13:20</td>
<td><strong>Correlation analysis of spectroscopic and biological features to follow mesenchymal stem cell differentiation</strong></td>
<td>Karolina Augustyniak¹, Hubert Latka¹, Monika Lesniak², Jacek Z. Kubiak², Robert Zdanowski³, Kamilla Malek¹</td>
<td>¹Jagiellonian University, Department of Chemical Physics, ²Military Institute of Medicine – National Research Institute, Laboratory of Molecular Oncology and Innovative Therapies</td>
</tr>
<tr>
<td>13:25-13:35</td>
<td><strong>Thriving Advantages of Drug Combination in Osteosarcoma Treatment – A Vibrational Microspectroscopy Study</strong></td>
<td>Raquel C. Laginha¹, Jéssica D. Silva¹, Maria Paula M. Marques¹, Gianfelice Cinque², Luís A. E. Batista de Carvalho¹, Ana L.M. Batista de Carvalho¹</td>
<td>¹Molecular Physical-Chemistry R&amp;D Unit, ²Diamond Light Source</td>
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<tr>
<td>Time</td>
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<td>Presentation</td>
<td>Authors</td>
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<tr>
<td>13:40-13:50</td>
<td>ATR-FTIR spectroscopic study of cells from the human monocytic cell line MONO-MAC-6 with stimulation by insulin</td>
<td>H. Michael Heise¹, Jacinta Tomas Borges¹, Yannik Merx¹, Saskia Simon¹, Sandra Stoppelkamp¹</td>
<td>¹SOUTH-WESTPHALIA UNIVERSITY OF APPLIED SCIENCES</td>
</tr>
<tr>
<td>13:55-14:05</td>
<td>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</td>
<td>Valentina Notarstefano¹, Alessia Belloni¹, Paolo Mariani¹, Elisabetta Giorgini¹, Hugh J. Byrne²</td>
<td>¹Marche Polytechnic University ²Technological University Dublin</td>
</tr>
<tr>
<td>14:10-14:20</td>
<td>Multimodal Spectroscopic Imaging (MALDI MSI vs Raman imaging / FTIR) in the analysis of the secondary metabolites</td>
<td>Mikolaj Krysa¹, Katarzyna Suśniak², Monika Szymańska-Chargot³, Anna Sroka-Bartrnica¹</td>
<td>¹Independent Unit of Spectroscopy and Chemical Imaging, Biomedical Faculty, Medical University of Lublin ²Independent Unit of Spectroscopy and Chemical Imaging, Biomedical Faculty, Medical University of Lublin; ³Department of Genetics and Microbiology, Institute of Biological Sciences, Maria Curie-Sklodowska University ³Institute of Agrophysics, Polish Academy of Sciences</td>
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<td>Multimodal Spectroscopic Imaging (MALDI MSI vs Raman imaging / FTIR) in the analysis of the secondary metabolites</td>
<td>Mikolaj Krysa¹, Katarzyna Suśniak², Monika Szymańska-Chargot³, Anna Sroka-Bartrnica¹</td>
<td>¹Independent Unit of Spectroscopy and Chemical Imaging, Biomedical Faculty, Medical University of Lublin; ³Department of Genetics and Microbiology, Institute of Biological Sciences, Maria Curie-Sklodowska University ³Institute of Agrophysics, Polish Academy of Sciences</td>
</tr>
<tr>
<td>14:30-15:00</td>
<td>Spectroscopic analysis of cancer-derived small extracellular vesicles for in vitro cancer diagnosis</td>
<td>Yuling Wang¹, Wei Zhang¹</td>
<td>¹Macquarie University</td>
</tr>
<tr>
<td>15:00-16:15</td>
<td>SESSION 3</td>
<td>A1-01</td>
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<tr>
<td>15:00-15:10</td>
<td>In-cell IR Difference Spectroscopy as a Time-resolved Method to Study Proteins in Living Cells</td>
<td>Lukas Goett-Zink¹, Anna Toschke¹, Eileen Baum¹, Tilman Kottke¹</td>
<td>¹Bielefeld University / Biophysical Chemistry and Diagnostics</td>
</tr>
<tr>
<td>15:15-15:25</td>
<td>Nanosecond time-resolved IR spectroscopy on proteins using quantum cascade laser setups</td>
<td>Jessica Klocke¹, Tilman Kottke¹</td>
<td>¹Biophysical Chemistry and Diagnostics, Bielefeld University</td>
</tr>
<tr>
<td>15:30-15:40</td>
<td>Rapidly determining the 3D structure of proteins by Surface-enhanced Raman spectroscopy</td>
<td>Hao Ma¹, Bin Ren¹</td>
<td>¹Xiamen University</td>
</tr>
<tr>
<td>15:45-15:55</td>
<td>Decoding early signs of erythrocyte pathology through analysis of protein secondary structure alterations</td>
<td>Tetiana Stepanenko¹, Katarzyna Bułat², Natalia Wilkosz², Fatih C. Alcikek³, Jakub Dybas⁴, Katarzyna M. Marzec⁵</td>
<td>¹Jagiellonian University, National Synchrotron Radiation Centre SOLARIS ²Łukasiewicz Research Network, Krakow Institute of Technology ³Goethe University, Institute for Cardiovascular Physiology ⁴Jagiellonian 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</td>
</tr>
<tr>
<td>16:00-16:10</td>
<td>Hydration Structure of Biomaterials Studied by Infrared Spectroscopy and Chemometrics</td>
<td>Shigeaki Morita¹</td>
<td>¹Osaka Electro-Communication University</td>
</tr>
<tr>
<td>15:00-15:15</td>
<td>In-situ study of nanocatalytic reactions using surface-enhanced Raman spectroscopy</td>
<td>Hua Zhang¹</td>
<td>¹College of Materials Xiamen University</td>
</tr>
<tr>
<td>15:20-15:35</td>
<td>Precision reusable flow SERS for Healthcare BioSensors 2.0</td>
<td>Jeremy Baumberg¹</td>
<td>¹University of Cambridge</td>
</tr>
<tr>
<td>Time</td>
<td>Title</td>
<td>Authors</td>
<td>Affiliations</td>
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<tr>
<td>15:40-15:50</td>
<td>Exciton-Phonon Coupling in MoSe2/WSe2 Heterobilayers Probed Using Resonant Raman Spectroscopy</td>
<td>Oisín Garrity(^1), Thomas Brumme(^2), Annika Bergmann(^3), Tobias Korn(^2), Patryk Kusch(^1), Stephanie Reich(^1)</td>
<td>(^1)Freie Universität Berlin (^2)Technische Universität Dresden (^3)Universität Rostock</td>
</tr>
<tr>
<td>15:55-16:05</td>
<td>In-Situ Cost-effective Methods for Fabricating SERS Substrates using Polydopamine</td>
<td>Ahmed Mahmoud(^1), Alexandra Teixeira(^1), Maria Sousa-Silva(^1), Sara Abalde-Cela(^1), Lorena Diéguez(^1)</td>
<td>(^1)The International Iberian Nanotechnology Laboratory (INL)</td>
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<td>16:10-16:20</td>
<td>Vanadium oxide nanoparticles as non-plasmonic platforms for surface-enhanced Raman spectroscopy</td>
<td>Eva Kočišová(^1), Anna Kuzminova(^2), Marek Procházka(^1), Ondřej Kylián(^2)</td>
<td>(^1)Institute of Physics, Faculty of Mathematics and Physics, Charles University (^2)Department of Macromolecular Physics, Faculty of Mathematics and Physics, Charles University</td>
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<tr>
<td>A0-04</td>
<td>(F) Advances in instrumentation</td>
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<td>15:00-15:15</td>
<td>Through the looking glass: Raman imaging through the bottle</td>
<td>Kishan Dholakia(^1)</td>
<td>(^1)University of Adelaide</td>
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<td>15:20-15:35</td>
<td>New Approaches for Raman Spectroscopic Imaging and High-Throughput Monitoring in Biomedical Applications</td>
<td>Torsten Frosch(^1)</td>
<td>(^1)Technical University Darmstadt</td>
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<td>15:40-15:50</td>
<td>Mode Optimized Tip-Enhanced Raman Scattering</td>
<td>Tao Chen(^1), Wei Wang(^1), Volker Deckert(^1)</td>
<td>(^1)Friedrich-Schiller University</td>
</tr>
<tr>
<td>15:55-16:05</td>
<td>Electric-field-dependent infrared nanospectroscopy of PVDF with an atomic force microscope</td>
<td>Maria Eleonora Temperini(^1), Valeria Giliberti(^2), Tommaso Venanzi(^2), Raffaella Polito(^1), Antonia Intze(^1), Michele Ortolani(^1)</td>
<td>(^1)Sapienza University of Rome</td>
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<td>16:10-16:20</td>
<td>Detection of microplastics using optical manipulation techniques and Raman spectroscopy</td>
<td>Silvie Bernatová(^1), Martin Kizovský(^1), Antonino Foti(^2), Maria Donato(^2), Pavel Zemánek(^1), Ota Samek(^1), Onofrio Maragò(^1), Jan Ježek(^1), Pietro Gucciardi(^2)</td>
<td>(^1)Institute of Scientific Instruments of the Czech Academy of Sciences (^2)Istituto per Processi Chimico-Fisici – Consiglio Nazionale delle Ricerche</td>
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<td>A0-03</td>
<td>(G) Analytical applications</td>
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<td>15:00-15:10</td>
<td>Chemically-specific in situ coherent Raman imaging of liquid-liquid phase separation in the crystallization process of pharmaceutical solids</td>
<td>Alba Arbiol(^1), Laurin Zöller(^2), Teemu Tomberg(^1), Jukka Saarinen(^1), Tom Konings(^1), Sara Carlert(^2), Eva Karlsson(^2), Anders Borde(^2), Quentin Vicentini(^2), Christoph Saal(^1), Jennifer Dressman(^2), Clare Strachan(^1)</td>
<td>(^1)Division of Pharmaceutical Chemistry and Technology, Vítkovická 5E, 00014 University of Helsinki, Finland (^2)Fraunhofer Institute for Translational Medicine and Pharmacology ITMP, Germany (^3)AstraZeneca R&amp;D Mölndal, S-431 83 Mölndal, Sweden</td>
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<td>15:15-15:25</td>
<td>Spectral identification of therapeutic allergen products</td>
<td>Christian Ickes(^1), Pirya Rani(^2), Kristiyana Tsenova(^3), Johanna Rost(^1), Frank Führer(^4), Detlef Bartel(^1), Christel Kamp(^1)</td>
<td>(^1)Paul-Ehrlich-Institut (^2)Saarland University (^3)Goethe University</td>
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| 15:30-15:40  | Raman-based Detection of Antibiotics and Metabolites in Pharmaceutical Formulations and Clinical-relevant Matrices  
Chen Liu1, Jürgen Popp1, Dana Cialla-May2  
1Institute 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  
2Leibniz 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 Tyagi1, Zain Ahmed1, Joao Cabral1, Sergei Kazarian1  
1Imperial College London |
| 16:05-16:15  | Rare earth-citrate complexes study using surface-enhanced Raman scattering spectra  
Hao Jin1, Tamitake Itoh2, Yuko. S. Yamamoto1  
1School of Materials Science, Japan Advanced Institute of Science and Technology  
2Nano-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**

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<th>Time</th>
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| 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 Iwata1  
1Gakushuin 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 Kim1  
1Department 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 Hellwig1, Tatjana Gerasimova2, Ana Filipa Seica Santos2, Thorsten Friedrich4  
1University of Strasbourg CNRS, UMR 7140  
2University of Strasbourg and University of Freiburg  
3University of Strasbourg, UMR 7140  
4University of Freiburg, Institute for Biochemistry |
| 11:05-11:20  | Local Structural Dynamics of Membrane Protein Bacteriorhodopsin Revealed by 2D Vibrational Spectroscopy  
Jianping Wang1  
1Institute of Chemistry |
| 11:25-11:35  | Plasmonic infrared study of SARS COV-2 mPro dimerization and its inhibition  
Federica Piccirilli1, Giovanni Birarda1, Lisa Vaccari1, Hendrik Vondracek1, Lucia Silvestini2, Francesco Spinozzi2, Paolo Mariani2, Antonio Palumbo Piccionello2, Vincenzo Aglieri3, Andrea Toma1, Maria Grazia Ortore1  
1Elettra Sincrotrone Trieste  
2Università politecnica delle Marche  
3Università Politecnica delle Marche  
4Università degli studi di Palermo  
5Istituto Italiano di tecnologia |
11:40-11:50  The chemical structure and conformation of tau protein aggregates at the growth phase
Kamila Sofińska1, Sara Seweryn1, Katarzyna Skirlińska-Nosek1, Piotr Batys2, Jakub Barbasz2, 
Ewelina Lipiec3
1Jagiellonian University, Faculty of Physics, Astronomy, and Applied Computer Science, 
M. Smoluchowski Institute of Physics 
2Jerzy 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 Fabris1, Chiara Deriu1, Kaleigh Scher2, Shaila Thakur1
1Politecnico di Torino 
2Rutgers University

11:05-11:20  Comparative study of p-Aminothiophenol adsorption by Surface-Enhanced Raman Spectroscopy
María Rosa López-Ramírez1, María De la Cabeza Fernández2, Alexis Alvar-Fernández2, 
Rafael Contreras-Cáceres2
1Department of Physical Chemistry, Faculty of Science, University of Málaga 
2Department of Chemistry in Pharmaceutical Sciences, Faculty of Pharmacy, Universidad 
Complutense de Madrid 
3Department 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 Królakowska1, Marcin Witkowski1, Lasse Jensen2, Wojciech Dzwolak1
1Faculty of Chemistry, University of Warsaw, Pasteura 1 
2Department 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 Yao1, Sadaf Ehtesabii1, Christiane Höppener1, Tanja Deckert-Gaudig1, Henrik Schneidewind1, 
Stephan Kupfer2, Stefanie Grüße2, Volker Deckert2
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 
3. 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 Pięta1, Aneta Kisielewska2, Ireneusz Piwoński2, Kamilla Małek1
1Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Krakow, Poland 
2Department 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 Kansiz2, Miriam Unger2, Deepthy Kavungal3, Felix Richter4, Hatice Altug5, Mark Anderson5
2Photothermal Spectroscopy Corp 
3Photothermal Spectroscopy Corp GmbH 
4Bionanophotonic Systems (BIOS) Laboratory & Lashuel Lab, EFPL 
5Bionanophotonic Systems (BIOS) Laboratory & Lashuel Lab, EPFL, 
6Caltech, Jet Propulsion Labs, NASA

11:00-11:10  Raman optical activity as a sensitive tool in analytical chemistry
Josef Kapitán1, Pavel Michal1, Jana Hudecová1, Petr Bouř2
1Palacký University Olomouc, Department of Optics 
2Institute of Organic Chemistry and Biochemistry, Academy of Sciences
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<th>Time</th>
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<th>Authors</th>
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<tr>
<td>11:15-11:25</td>
<td>A novel wide-field Raman imaging setup</td>
<td>B. J. A. Mooij¹, R. W. Schmidt¹, W. A. J. Vijvers², F. Ariese¹</td>
<td>¹LaserLaB, Vrije Universiteit Amsterdam ²Chromodynamics B.V.</td>
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<tr>
<td>11:30-11:40</td>
<td>Simultaneous co-located Raman and SEM imaging for correlated SEM microscopy</td>
<td>Jorge Diniz¹, Agnieszka Sozanska², Tim Batten³</td>
<td>¹Renishaw plc ²Renishaw Spzoo ³Renishaw PLC</td>
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<td>11:45-11:55</td>
<td>Reducing frequency fluctuations induced by back-reflected light into a non-stabilized low cost laser diode</td>
<td>Konstantinos Stergiou¹, Oleksii Ilichenko², Yurii Pilhun¹, Andrii Kutsyk²</td>
<td>¹Lightnovo ApS ²Technical University of Denmark</td>
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<td>12:00-12:10</td>
<td>Maximizing Positive Microplastic Particle Identification and Provenance Through Optimized Optical and Raman Microscopy – Particle-Correlated Raman Spectroscopy (PCRS)</td>
<td>Andrew Whitley¹, Eunah Lee¹, Massimiliano Rocchia¹, Sebastien Laden¹</td>
<td>¹HORIBA</td>
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<td>(G) Analytical applications</td>
<td>Chair: Entesar Al-Hetlani</td>
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<td>10:45-10:55</td>
<td>Silicon within fossil and cultivated coccoliths of Helicosphaera carteri: new insights from Infrared Spectromicroscopy and X-ray Fluorescence analyses</td>
<td>Giovanni Birarda¹, Manuela Bordiga², Diana Eva Bedolla³, Alessandra Gianoncelli¹, Simone Pollastri¹, Valentina Bonanni¹, Gianluca Gariani¹, Lisa Vaccari², Federica Cerino², Marina Cabrini², Alfred Beran², Mario Zanoni², Maurizio Zuccotti², Giulia Fiorentino², Miriam Cobianchi², Andrea Di Giulio², Claudia Lupi²</td>
<td>¹Elettra—Sincrotrone Trieste ²National Institute of Oceanography and Applied Geophysics OGS ³AREA Science Park ⁴Department of Biology and Biotechnologies “Lazzaro Spallanzani”, University of Pavia ⁵Department of Earth and Environmental Sciences, University of Pavia</td>
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<td>11:00-11:10</td>
<td>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</td>
<td>Joanna Chwiej¹, Natalia Janik-Olchawa², Agnieszka Drózdz², Aleksandra Wajda², Maciej Sitarz¹, Daniel Horak², Michal Babic², Jolanta Gol¹, Zuzanna Setkowicz-Janeczko², Aleksandra Wilk¹, Marzena Rugieł¹, Katarzyna Matusiak¹, Christoph Sandt², Ferenc Borondics², Magdalena Wytrwat-Sarna³</td>
<td>¹AGH University of Krakow ²Jagiellonian University ³Maria Curie-Skłodowska University in Lublin ⁴Czech Academy of Sciences ⁵SOLEIL</td>
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<td>11:15-11:25</td>
<td>The increase of fibres and flavonoids concentration in the Zea mays stem treated with Nod-factor-based biofertilizer. A multimodal imaging study.</td>
<td>Mikolaj Krysa¹, Katarzyna Susniak², Cai Li Song³, Monika Szymanska-Chargot⁴, Artur Zdunek⁴, Izabela S. Piate⁵, Janusz Podlesny⁴, Anna Sroka-Barnicka¹, Sergei G. Kazarian³, Izabela S. Piate⁵</td>
<td>¹Medical University of Lublin, Independent Unit of Spectroscopy and Chemical Imaging, ²Maria Curie-Skłodowska University, Department of Genetics and Microbiology ³Imperial Collage London, Department of Chemical Engineering ⁴Institute of Agrophysics, Polish Academy of Sciences ⁵Institute of Physical Chemistry, Polish Academy of Sciences ⁶Institute of Soil Science and Plant Cultivation, State Research Institute</td>
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<td>11:30-11:40</td>
<td>Development of Raman Spectroscopic analysis techniques to assess quality biomarkers in fish</td>
<td>Jeremy Landry¹, Peter Torley¹, Ewan Blanch¹</td>
<td>¹RMIT University</td>
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<td>11:45-11:55</td>
<td>Visualization and identification of components in a gigantic spherical dolomite concretion by Raman imaging and MCR analysis</td>
<td>Ryosuke Kitanaka¹, Motohiro Tsuboi², Tomoko Numata³, Yusuke Muramiya⁴, Hidekazu Yoshida⁵, Yukihiro Ozaki²</td>
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<td>¹Kwansei Gakuin University ²Kwansei Gakuin University ³HORIBA Techno Service Co. Ltd. ⁴Fukada Geological Institute ⁵Nagoya University</td>
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<td>12:00-12:10</td>
<td>SIP vibrational microspectroscopy in micro-structured chips reveals single-cell metabolic dynamics of soil microbes</td>
<td>Milda Pucetaite¹, Edith C. Hammer¹, Louise C. Andersen², Sofía Gabriela Rodas Samayo²</td>
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<td>¹Department of Biology, Lund University ²Department of Earth Science, University of Gothenburg</td>
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<td>A0-01</td>
<td>(H) Biodiagnostic spectroscopy</td>
<td>Chair: Nick Stone</td>
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<td>10:45-11:00</td>
<td>High-resolution Raman imaging of &gt;300 cells from human patients affected by nine different leukemia subtypes: a global clustering approach</td>
<td>Renzo Vanna¹, Andrea Masella², Manuela Bazzarelli³, Paola Ronchi³, Aufried Lenferink⁴, Cristina Tresoldi⁵, Carlo Morasso⁶, Marzia Bedoni⁶, Dario Polli⁶, Fabio Ciciri⁷, Giulia De Polli⁷, Matteo Bregonzio⁸, Ces dances Otto⁹</td>
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<td>¹Istituto di Fotonica e Nanotecnologie – Consiglio Nazionale delle Ricerche (IFN-CNR) ²3rdPlace SRL ³IRCCS Ospedale San Raffaele ⁴University of Twente ⁵IRCCS Istituti Clinici Scientifici Maugeri ⁶IRCCS Fondazione Don Carlo Gnocchi ⁷Politecnico di Milano</td>
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<td>11:05-11:20</td>
<td>Surface Enhanced Spatially Offset Raman Spectroscopy: A Promising Optical Imaging Modality in Preclinical Cancer Imaging</td>
<td>Fay Nicolson¹, Eunah Lee², Andrew Whitely², Bohdan Andreiuk², Scott Rudder³, Samuel Mabbott⁴, Kevin Haigis⁵</td>
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<td>¹Dana-Farber Cancer Institute ²HORIBA Scientific ³Dana-Farber Cancer Insitute ⁴Opto-Sigma ⁵Texas A&amp;M University</td>
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<td>11:25-11:35</td>
<td>Surface-enhanced Raman Spectroscopy in tumor detection</td>
<td>Aneta Kowalska¹, Marta Czaplicka¹, Ariadna Nowicka², Tomasz Szymborski³, Izabela Chmielewska⁴, Wojciech Kukwa³, Agnieszka Kamińska³</td>
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<td>¹Institute of Physical Chemistry Polish Academy of Sciences ²Institute for materials Research and Quantum Engineering, Poznań University ³Institute of Physical Chemistry, Polish Academy of Sciences ⁴Department of Pneumonology, Oncology and Allergology, Medical University of Lublin ⁵Szpital Czerniakowski, Medical University of Warsaw</td>
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<td>11:40-11:50</td>
<td>FTIR Spectroscopy for Bladder Carcinoma Detection and Prediction of Grade, Invasion, and Lymph Nodes Metastases</td>
<td>Monika Kujdowicz¹, David Perez-Guita², Piotr Chlosta³, Krzysztof Okon⁴, Kamilla Malek⁵</td>
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<td>¹Department of Patomorphology, Jagiellonian University Medical College; Faculty of Chemistry, Jagiellonian University ²Department of Analytical Chemistry, University of Valencia ³Department of Urology, Jagiellonian University Medical College ⁴Department of Patomorphology, Jagiellonian University Medical College ⁵Faculty of Chemistry, Jagiellonian University</td>
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### Raman Spectroscopic application in cervical cancer screening

Rubina Shaikh, Aoife Mc Guinness, Alison Malkin, John O’Leary, Cara Martin, Fiona Lyng

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, Grangegorman, Ireland

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

TCD CERVIVA Molecular Pathology Laboratory, The Coombe Women and Infants University Hospital, Dublin, Ireland. 5. Trinity St James Cancer Institute, Trinity College Dublin, Ireland

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### 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

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, Iona Ivalo, Rory Cowin, Martin Appleby, Catherine Royle, Igor Sazanovich, Dimitri Chekulaev, Anthony Meijer, Alexander Auty, Guaznhi Wu, Tao Cheng, James Shipp

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, Subashani Maniam, Nilamuni De Silva, Helmut Huegel, Ewan Blanch

1. RMIT University

#### 11:00-11:10
**State of water in various environments: aliphatic ketones. MIR/NIR spectroscopic, dielectric and theoretical studies**

Mirosław Zmarzły, Krzysztof Bet, Justyna Grabska, Christian Huck, Sylwester Mazurek

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, Grzegorz Zając, Monika Halat, Takumi Tani, Tomotsumi Fujisawa, Masashi Unno

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
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<td>11:30-11:40</td>
<td>Evaluating the acidity levels in super-acidic ionic liquids by Raman Spectroscopy</td>
<td>Cedric Malherbe¹</td>
<td>University of Liège</td>
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| 11:45-11:55 | Unraveling the Structural Polymorphism of Mononucleotide G-Quadruplexes via Raman Optical Activity | Stépán Jílek¹, Josef Kapitán², Mohammed Siddique Para Kkadan¹, Ivan Barvík¹, Václav Profant¹ | Institute of Physics, Faculty of Mathematics and Physics, Charles University  
Department of Optics, Faculty of Science, Palacký University Olomouc |
| A1-02    | (E) Nonlinear vibrational spectroscopy                               |                                                                                             |                                                                            |
| 10:45-11:00 | Proteins at charged biointerfaces as revealed by nonlinear vibrational spectroscopy | Zsuzsanna Heiner¹                          | Humboldt-Universität zu Berlin, SALSA                                       |
| 11:05-11:20 | Time-domain Raman spectroscopy for large-scale cell screening        | Kotaro Hiramatsu¹                           | The University of Tokyo                                                 |
| 11:25-11:35 | Good vibrations: small molecule raman optical probes to image metabolism in tissue microenvironments | Ailsa Geddis¹, Fabio De Moliner¹, Colin Campbell¹, Marc Vendrell¹ | 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 Madzharova², Adam Chatterley³, Steven Roeters¹, Tobias Weidner³ | Aarhus University                                                       |
| 11:55-12:05 | Molecular structure, surface charge and dissolution of the MgO-water interface influenced by liquid flow | Moritz Zelenka¹, Ellen H. G. Backus¹ | University of Vienna                                           |
| A0-04    | (F) Advances in instrumentation                                      |                                                                                             |                                                                            |
| 10:45-11:00 | New Perspectives for Mid-IR Spectroscopy of Liquids as Enabled by Quantum Cascade Lasers | Bernhard Lendl¹, Alicja Dabrowska¹, Daniel-ralph Hermann¹, Giovanna Ricchiuti¹, Gustavo Lukasievicz², Georg Ramer¹ | TU Wien                                                                  |
| 11:05-11:20 | Stimulated Raman scattering and resonance Raman spectroscopy combined with holography, interferometry and video imaging | Kerstin Ramser¹                           | Department of Engineering Sciences and Mathematics/Luleå University of Technology |
| 11:25-11:35 | Developing Sensitive Stimulated Raman Scattering (SRS) Microscopy    | Krzysztof Brzozowski¹, Anna Pieczara², Małgorzata Baranska³ | Jagiellonian University  
Jagiellonian Centre for Experimental Therapeutics  
Jagiellonian University, Jagiellonian Centre for Experimental Therapeutics |
| 11:40-11:50 | Rapid field-resolved infrared fingerprinting and discrimination of particles in flow | Marinus Huber¹, Daniel Gerz¹, Holger Mirkes², Florian Lindinger², Yannick Münzenmaier², Alexander Weigel³, Mark Kielpinski³, Thomas Henkel¹, Mihaela Zigman⁵, Ferenc Krausz⁵, Jürgen Popp¹, Ioachim Pupeza¹ | Leibniz Institute of Photonic Technology  
Ludwig Maximilians University  
Max Planck Institute of Quantum Optics |
<p>| 11:55-12:05 | Current state of spectrometer miniaturization: synergy with analytical potential of NIR spectroscopy | Christian W. Huck¹, Justyna Grabska¹, Krzysztof B. Bec¹ | University of Innsbruck                                               |</p>
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<td>10:45-11:00</td>
<td>A0-03 (G)</td>
<td>Probing chemical speciation with low-frequency Raman spectroscopy</td>
<td>Keith Gordon&lt;sup&gt;1&lt;/sup&gt; &lt;br&gt; &lt;sup&gt;1&lt;/sup&gt;University of Otago and Dodd Walls Centre – Te Whai Ao</td>
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<tr>
<td>11:05-11:20</td>
<td>A0-03</td>
<td>Profiling of Human Bones by Vibrational Spectroscopy</td>
<td>Maria Paula Marques&lt;sup&gt;1&lt;/sup&gt;, David Gonçalves&lt;sup&gt;2&lt;/sup&gt;, Stewart F. Parker&lt;sup&gt;3&lt;/sup&gt;, Winfried Kockelmann&lt;sup&gt;2&lt;/sup&gt;, Giulia Festa&lt;sup&gt;4&lt;/sup&gt;, Luís Batista de Carvalho&lt;sup&gt;1&lt;/sup&gt; &lt;br&gt; &lt;sup&gt;1&lt;/sup&gt;Univ. Coimbra, Molecular Physical-Chemistry R&amp;D Unit &lt;br&gt; &lt;sup&gt;2&lt;/sup&gt;Archaeosciences Lab., Directorate General Cultural Heritage &lt;br&gt; &lt;sup&gt;3&lt;/sup&gt;ISIS Facility, STFC Rutherford Appleton Laboratory &lt;br&gt; &lt;sup&gt;4&lt;/sup&gt;CREF – Museo Storico della Fisica e Centro Studi e Ricerche Enrico Fermi</td>
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<td>11:25-11:35</td>
<td>A0-03</td>
<td>Fusion of IR and RS spectral data in 2D and 3D in vitro studies for the spheroid blood-brain barrier model</td>
<td>Anna Antolak&lt;sup&gt;1&lt;/sup&gt;, Aleksandra Pragnąca&lt;sup&gt;2&lt;/sup&gt;, Zuzanna Krysiak&lt;sup&gt;3&lt;/sup&gt;, Monika Leśniak&lt;sup&gt;2&lt;/sup&gt;, Joanna Korszun&lt;sup&gt;4&lt;/sup&gt;, Robert Zdanowski&lt;sup&gt;1&lt;/sup&gt;, Kamilla Malek&lt;sup&gt;1&lt;/sup&gt; &lt;br&gt; &lt;sup&gt;1&lt;/sup&gt;Jagiellonian University &lt;br&gt; &lt;sup&gt;2&lt;/sup&gt;Jagiellonian University, Doctoral School of Exact and Natural Sciences &lt;br&gt; &lt;sup&gt;3&lt;/sup&gt;Military Institute of Medicine National Research Institute &lt;br&gt; &lt;sup&gt;4&lt;/sup&gt;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</td>
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<td>11:40-11:50</td>
<td>A0-03</td>
<td>Aging in coronal dentine of the human tooth seen at the sub-micron resolution in non-contact IR spectroscopy</td>
<td>Agnieszka Banas&lt;sup&gt;1&lt;/sup&gt;, Krzysztof Banas&lt;sup&gt;1&lt;/sup&gt;, Chin-ying, Stephen Hsu&lt;sup&gt;2&lt;/sup&gt;, Guang Rong Tang&lt;sup&gt;2&lt;/sup&gt;, Mark B.H. Breese&lt;sup&gt;1&lt;/sup&gt; &lt;br&gt; &lt;sup&gt;1&lt;/sup&gt;Singapore Synchrotron Light Source NUS &lt;br&gt; &lt;sup&gt;2&lt;/sup&gt;National University of Singapore, Dentistry Department</td>
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<td>11:55-12:05</td>
<td>A0-03</td>
<td>Micro and nano-spectroscopic studies of modified metallic surface for implantology application</td>
<td>Dominika Święch&lt;sup&gt;1&lt;/sup&gt;, Gaetano Palumbo&lt;sup&gt;1&lt;/sup&gt;, Natalia Piergies&lt;sup&gt;2&lt;/sup&gt;, Kamila Kollbek&lt;sup&gt;3&lt;/sup&gt;, Czesława Paluszkiewicz&lt;sup&gt;2&lt;/sup&gt; &lt;br&gt; &lt;sup&gt;1&lt;/sup&gt;AGH University of Science and Technology, Faculty of Foundry Engineering, av. Mickiewicza 30 &lt;br&gt; &lt;sup&gt;2&lt;/sup&gt;Institute of Nuclear Physics Polish Academy of Sciences &lt;br&gt; &lt;sup&gt;3&lt;/sup&gt;AGH University of Science and Technology, Academic Centre for Materials and Nanotechnology, av. Mickiewicza 30</td>
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<td>10:45-11:00</td>
<td>A0-01 (H)</td>
<td>Portable Raman spectroscopy for in-clinic skin and prostate cancer diagnosis</td>
<td>Suse J. Van Breugel&lt;sup&gt;1&lt;/sup&gt;, Hannah Matthews&lt;sup&gt;2&lt;/sup&gt;, Kamran Zargar-Shoshtari&lt;sup&gt;3&lt;/sup&gt;, Paul Jarret&lt;sup&gt;3&lt;/sup&gt;, Michelle Locke&lt;sup&gt;3&lt;/sup&gt;, Cather Simpson&lt;sup&gt;1&lt;/sup&gt;, Michel Nieuwoudt&lt;sup&gt;1&lt;/sup&gt;, Claude Aguergaray&lt;sup&gt;4&lt;/sup&gt; &lt;br&gt; &lt;sup&gt;1&lt;/sup&gt;The University of Auckland &lt;br&gt; &lt;sup&gt;2&lt;/sup&gt;Counties Manukau District Health Board &lt;br&gt; &lt;sup&gt;3&lt;/sup&gt;Department of Dermatology, Middlemore Hospital &lt;br&gt; &lt;sup&gt;4&lt;/sup&gt;Department of Plastic Surgery, Middlemore Hospital</td>
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<td>11:05-11:20</td>
<td>A0-01</td>
<td>Self-assembled nanogap arrays of gold nanoparticles in dimple nanopores induced by DNA hybridization</td>
<td>Hajun Dang&lt;sup&gt;1&lt;/sup&gt;, Jaebum Choo&lt;sup&gt;2&lt;/sup&gt; &lt;br&gt; &lt;sup&gt;1&lt;/sup&gt;Chung-Ang University</td>
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<td>11:25-11:35</td>
<td>A0-01</td>
<td>An injectable biosensor for continuous remote monitoring of patients with prostate cancer</td>
<td>Marta Aranda Palomer&lt;sup&gt;1&lt;/sup&gt;, Maria S. Relvas&lt;sup&gt;2&lt;/sup&gt;, Sergio Quintero&lt;sup&gt;4&lt;/sup&gt;, Jason B. King&lt;sup&gt;3&lt;/sup&gt;, Mengkun Chen&lt;sup&gt;3&lt;/sup&gt;, James W. Tunnell&lt;sup&gt;2&lt;/sup&gt;, Ana Oliveira&lt;sup&gt;4&lt;/sup&gt;, Pedro Costa&lt;sup&gt;3&lt;/sup&gt;, Rui Sousa&lt;sup&gt;2&lt;/sup&gt;, Adriana Mendes&lt;sup&gt;3&lt;/sup&gt;, Olga Martinho&lt;sup&gt;3&lt;/sup&gt;, Fatima Baltazar&lt;sup&gt;6&lt;/sup&gt;, Lorena Dieguez&lt;sup&gt;3&lt;/sup&gt;, Sara Abalde-Cela&lt;sup&gt;1&lt;/sup&gt; &lt;br&gt; &lt;sup&gt;1&lt;/sup&gt;International Iberian Nanotechnology Laboratory (INL) &lt;br&gt; &lt;sup&gt;2&lt;/sup&gt;International Iberian Nanotechnology laboratory (INL) &lt;br&gt; &lt;sup&gt;3&lt;/sup&gt;University of Texas at Austin (UTA) &lt;br&gt; &lt;sup&gt;4&lt;/sup&gt;Stemmaters Biotecnologia e Medicina Regenerativa SA &lt;br&gt; &lt;sup&gt;5&lt;/sup&gt;Stemmaters Biotecnologia e Medicina Regenerativa &lt;br&gt; &lt;sup&gt;6&lt;/sup&gt;Life and Health Research Institute (ICVS)</td>
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<td>11:40-11:50</td>
<td>Dual nano-heater and SERS temperature sensor for cancer photothermal therapy</td>
<td>William H. Skinner¹, Renata L. Sala², Kamil Sokolowski², Jeremy J. Baumberg², Oren A. Scherman², Benjamin Gardner², Pavel Matousek³, Nicholas Stone³</td>
<td>¹University of Exeter, ²University of Cambridge, ³STFC Rutherford Appleton Laboratory</td>
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<tr>
<td>11:55-12:05</td>
<td>Blood pulse dynamics investigation with non-invasive Raman spectroscopy</td>
<td>Maciej Wróbel¹</td>
<td>¹Gdansk University of Technology</td>
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<td>12:10-13:10</td>
<td>Lunch</td>
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<td>13:10-14:30</td>
<td>SESSION 2</td>
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<td>A1-01</td>
<td>(I) Chemometrics&amp;machine learning</td>
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<td>13:10-13:25</td>
<td>Two-trace two-dimensional (2T2D) FTIR correlation spectra applied as input</td>
<td>Bogumila Kupcewicz¹</td>
<td>¹Nicolaus Copernicus University, Faculty of Pharmacy</td>
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<td>13:30-13:40</td>
<td>Decoupling of morphological and chemical information in µFTIR spectra using deep learning</td>
<td>Uladzislau Blazhko¹, Eirik Magnussen¹, Johanne Solheim¹, Simona Dzurendova¹, Volha Shapaval¹, Achim Kohler¹</td>
<td>¹Norwegian University of Life Sciences</td>
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<td>13:45-13:55</td>
<td>Investigation of the bread aging process by handheld NIR spectroscopy in tandem with 2D-COS and MCR-ALS analyses</td>
<td>Marina De Géa Neves¹, Isao Noda², Heinz Wilhelm Siesler¹</td>
<td>¹Department of Physical Chemistry, University Duisburg-Essen, ²Department of Materials Science and Engineering, University of Delaware</td>
</tr>
<tr>
<td>14:00-14:10</td>
<td>Can we follow the metabolism of single leukemic cells using Raman spectroscopy?</td>
<td>Anna M. Nowakowska¹, Aleksandra Borek-Dorosz¹, Patrycja Dawiec², Patrycja Leszczenko², Adriana Adamczyk², Kacper Siakala¹, Justyna Jakubowska¹, Marta Zabczynska¹, Agata Pastorczyk³, Kinga Ostrowska³, Wojciech Mlynarski², Małgorzata Baranska², Katarzyna Majzer¹</td>
<td>¹Jagiellonian University in Krakow, Faculty of Chemistry, Department of Chemical Physics, Krakow, Poland, ²Jagiellonian University in Krakow, Faculty of Chemistry, Department of Chemical Physics, Krakow, Poland, ³Doctoral School of Exact and Natural Sciences, Jagiellonian University, Krakow, Poland</td>
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<td>A1-02</td>
<td>(E) Nonlinear vibrational spectroscopy</td>
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<td>13:10-13:25</td>
<td>Specific Ion Effects in the Electrical Double Layer Structure at the Silica/Aqueous Interface</td>
<td>Julianne Gibbs¹, Nathaniel Tetteh¹, Shyam Parshotam¹</td>
<td>¹University of Alberta</td>
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<tr>
<td>13:30-13:45</td>
<td>Mechanistic Approach to Investigate the Water Evaporation Process at Air/Water Interface using Hofmeister Ions</td>
<td>Bhawna Rana¹, David J. Fairhurst², Kailash C. Jena¹</td>
<td>¹Indian Institute of Technology Ropar, ²Nottingham Trent University</td>
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<td>13:50-14:00</td>
<td>Ultrafast decay of coupled molecule-plasmon nanogap structure</td>
<td>Fiona Bell¹, Lukas Jakob¹, Ishaan Lohia¹, Rakesh Arul¹, Jeremy Baumberg¹</td>
<td>¹University of Cambridge</td>
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<tr>
<td>14:05-14:15</td>
<td>How and when does the collapse of a macromolecule in water start? From time-resolved Raman to elastic light scattering viewpoint.</td>
<td>Marcin Pastorczak², Michał Nejbauer², Naoki Shinyashiki², Masanobu Takatsuka², Gonzalo Angulo¹, Yuriy Stepanenko³, Cezław Radzewicz³</td>
<td>¹Institute of Physical Chemistry Polish Academy of Sciences, ²Department of Physics, School of Science, Tokai University, ³Institute of Experimental Physics, Faculty of Physics, University of Warsaw</td>
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14:20-14:30 Taking Advantage of High Sensitivity Enabled by Stimulated Raman Scattering: Multi-Parameter Analysis of Nanoplastics in Flow
Maximilian Huber1, Liron Zada2, Freek Ariese2, Natalia P. Ivleva1
1Technical University of Munich, Institute of Water Chemistry, Chair of Analytical Chemistry and Water Chemistry, School of Natural Sciences (Dep. Chemistry)
2Vrije Universiteit Amsterdam, LaserLaB Amsterdam, Department of Physics and Astronomy

AO-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 Dabrowska1, Bernhard Lendl1
1Technische Universität Wien

Ting-hao Chen1, Hirotugu Hiramatsu1
1Department 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 Ilchenko1, Yuri Pilhur2, Andrii Kutsyk1, Yaman Goksel1, Elodie Dumont2, Thomas Andersen3, Mikhail Lassen4, Hemanshu Mundhada5, Christian Jendresen6, Anja Boisen1
1Technical University of Denmark
2Lightnovo ApS
3Odense University Hospital
4Danish National Metrology Institute
5Cysbio ApS

13:55-14:05 A correlated OF2i®-Raman method for micro- and nanoparticle detection and chemical analysis in liquids
Christian Neuper1, Marko Šimić2, Christian Hill3, Werner Grogger4, Harald Fitzek5
1Graz Centre of Electron Microscopy, Steyrergasse 17, Austria / Brave Analytics GmbH, Austria
2Brave Analytics GmbH, Austria / Gottfried Schatz Research Center, Division of Biophysics, Medical University of Graz, Neue Stiftungstrasse 2, Graz 8010, Austria / Institute of Physics, University of Graz, Universitätsplatz 5, Graz 8010, Austria
3Brave Analytics GmbH, Austria / Gottfried Schatz Research Center, Division of Biophysics, Medical University of Graz, Neue Stiftungstrasse 2, Graz 8010, Austria
4Graz Centre of Electron Microscopy, Steyrergasse 17, Austria / Institute of Electron Microscopy and Nanoanalysis, NAWI Graz, Graz University of Technology, Steyrergasse 17, Austria
5Graz 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 Sacco1, Giulia Barzan1, Slavica Matić2, Chiara D&apos;apos;Errico, Marta Vallino2, Marina Ciuffo2, Emanuela Noris3, Andrea Mario Giovannozzi3, Chiara Portesi3, Andrea Mario Rossi3
1National Metrology Research Institute (INRiM)
2Institute 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 Lorent1, Sagie Katz2, Vladimir Pelmenschikov1, Giorgio Caserta1, Stefan Frielingsdorf1, Maria Alessandra Martin1, Konstantin Bikkave1, Ingrid Span3, James A.F. Birrell4, Oliver Lenz1, Marius Horch5, Ingo Zebger1
1Technische Universität Berlin, Insititut für Chemie
2Max-Planck-Institut für Chemische Energiekonversion
3Friedrich-Alexander-Universität Erlangen-Nürnberg
4University of Essex, School of Life Sciences
5Freie Universität Berlin, Institut für Physik, Biophysik

AO-03 (G) Analytical applications
Chair: Natalia Ivleva

Krzysztof B. Bec1, Justyna Grabska1, Jovan Badzoka1, Christian W. Huck1
1University of Innsbruck
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<td>13:25-13:35</td>
<td>Quantification of microplastics in environmental samples through a combination of optical and FTIR- and Raman microspectroscopy enhanced by Machine Learning evaluation</td>
<td>Dieter Fischer¹, Kristina Enders¹, Robin Lenz¹, Franziska Fischer², Elisavet Kanaki³, Julia Muche¹, Benedikt Hufnagl¹. ¹Leibniz-Institut für Polymerforschung Dresden, ²Advanced Mask Technology Center GmbH Dresden, ³Purency GmbH Wien.</td>
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<tr>
<td>13:40-13:50</td>
<td>Comparison of Raman- and fluorescence techniques for detection and identification of microplastics in environmental samples</td>
<td>Merel Konings¹, Liron Zada¹, Robert Schmidt¹, Freek Ariese¹. ¹Vrije Universiteit Amsterdam.</td>
</tr>
<tr>
<td>13:55-14:05</td>
<td>Applications of optical photothermal infrared spectroscopy (O-PTIR) in plastic pollution research: from detecting microplastics to monitoring the production of microbial bioplastic</td>
<td>Cassio Lima¹, Howbeer Muhamadali¹, Royston Goodacre¹. ¹University of Liverpool.</td>
</tr>
<tr>
<td>14:10-14:20</td>
<td>Nanoscale chemical characterization is crucial for polymer recycling</td>
<td>Georg Ramer¹, V. D. Dos Santos A. Catarina¹, Lena Neubauer², Bernhard Lendl². ¹TU Wien / Institute for chemical Technologies and Analytics, ²TU Wien / Institute for chemical Technologie and Analytics.</td>
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<tr>
<td>14:25-14:35</td>
<td>In-line near-infrared spectroscopic monitoring for injection molding of biodegradable polymer blends</td>
<td>Itsuki Yoshikawa¹, Yuta Hikima¹, Masahiro Ohshima¹. ¹Kyoto University.</td>
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**A0-01 (H) Biodiagnostic spectroscopy**

Chair: Peter Gardner

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<td>13:10-13:20</td>
<td>Rapid identification of bacteria isolated directly from patient urine and diagnosis of their antibiotic susceptibility using infrared spectroscopy-based machine learning</td>
<td>George Abu-Aqil¹, Manal Suleiman¹, Uraib Sharaha¹, Lior Nesher⁴, Itshak Lapidot¹, Ahmad Salman⁴, Mahmoud Huleilh⁴. ¹Ben-Gurion University of the Negev, ²Soroka University Medical Center, ³Afeka Tel-Aviv Academic College of Engineering, ⁴Shamoon College of Engineering.</td>
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<td>13:25-13:35</td>
<td>Supplementation of vitamin C and E – an effect on human gastrointestinal tract tissues and cells: Raman spectroscopy and imaging</td>
<td>Karolina Beton-Mysur¹, Beata Brożek-Płuska¹. ¹Lodz University of Technology, Faculty of Chemistry, Institute of Applied Radiation Chemistry, Laboratory of Laser Molecular Spectroscopy.</td>
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<tr>
<td>13:40-13:50</td>
<td>Molecular Characterisation of T-cell acute lymphoblastic leukemia using Raman spectroscopy</td>
<td>Patrycja Dawiec¹, Patrycja Leszczenko², Anna Nowakowska², Karolina Czuja², Justyna Jakubowska³, Marta Zabczyńska³, Agata Pastorczak³, Kinga Ostrowska³, Wojciech Młynarski³, Małgorzata Baranska³, Katarzyna Majzner³. ¹Jagiellonian University in Krakow, Faculty of Chemistry, Department of Chemical Physics, Doctoral School of Exact and Natural Sciences; ²Jagiellonian University in Krakow, Faculty of Chemistry, Department of Chemical Physics; ³Department of Pediatrics, Oncology and Hematology, Medical University of Lodz.</td>
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<td>13:55-14:05</td>
<td>Raman-based assessment of the endothelial response to antiretroviral drugs: in vitro studies on NNRTI-treated human endothelial cells</td>
<td>Jagoda Orleńska¹, Wiktoria Wiecek¹, Małgorzata Baranska², Katarzyna Majzner². ¹Jagiellonian University, Faculty of Chemistry, Department of Chemical Physics, Krakow, Poland; 2 Doctoral School of Exact and Natural Sciences, Jagiellonian University in Krakow, Krakow, Poland.</td>
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¹Jagiellonian University, Faculty of Chemistry, Department of Chemical Physics, Krakow, Poland; 2 Doctoral School of Exact and Natural Sciences, Jagiellonian University in Krakow, Krakow, Poland; 3 Jagiellonian University in Krakow, Jagiellonian Centre for Experimental Therapeutics (JCET), Krakow, Poland.
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<td>14:10-14:20</td>
<td>SESSION 3</td>
<td>Bladder Cancer detection by Fourier Transform Infrared Spectroscopy (FTIR) using urine samples.</td>
<td>Imane Oudahmane¹, Fayek Taha², Elie Sarkees³, Jade Vanmansart¹, Vincent Vuiblet³, Stéphane Larre², Olivier Piot¹</td>
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<td>¹BioSpecT (Translational BioSpectroscopy) EA 7506, Université de Reims Champagne-Ardenne.</td>
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<td>²Department of Urology, University Hospital of Reims.</td>
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<td>³Department of Biopathology, University Hospital of Reims.</td>
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<td>14:25-14:35</td>
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<td>Exploring the potential for Deep Raman Spectroscopy for non-invasive sex determination of chicken eggs</td>
<td>Leonard Van den Tweel¹, Freek Ariese², Carla Van der Pol³, Henry Van den Brand¹</td>
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<td>¹Adaptation Physiology Group, Wageningen University &amp; Research</td>
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<td>²LaserLab, Department of Physics and Astronomy, Vrije Universiteit Amsterdam</td>
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<td>³Research Department, HatchTech B.V.</td>
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<td>14:30-15:00</td>
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<td>Coffee Break</td>
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<td>15:00-15:15</td>
<td>SESSION 3</td>
<td>A1-01 (I) Chemometrics &amp; machine learning</td>
<td>Chair: Stefania Dana Iancu</td>
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<td>15:00-15:10</td>
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<td>Advancing cancer stem cell detection through line illumination Raman microscope and hydrogel substrate.</td>
<td>Jean-Emmanuel Clément¹, Zannatul Ferdous¹, Thomas Bocklitz², Katsumasa Fujita³, Jian Ping Gong¹,</td>
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<td>Shinya Tanaka¹, Tamiki Komatsuzaki³</td>
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<td>¹Hokkaido University-ICReDD</td>
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<td>²University of Bayreuth</td>
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<td>³Osaka University</td>
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<td>15:15-15:25</td>
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<td>Discrimination between chemoresistant and chemosensitive ovarian cancer cells with confocal Raman microscopy</td>
<td>Elina Harju¹, Teemu Tomberg¹, Sara Fraser-Miller², Jukka Saarinen¹, Kathleen J. Sircombe³,</td>
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<td>Sarah Hook¹, Keith C. Gordon², Clare J. Strachan¹</td>
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<td>¹Division of Pharmaceutical Chemistry and Technology, Faculty of Pharmacy, University of Helsinki</td>
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<td>²The Dodd-Walls Centre for Photonic and Quantum Technologies – Te Whai Ao and Department of Chemistry, University of Otago</td>
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<td>³School of Pharmacy, University of Otago</td>
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<td>15:30-15:40</td>
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<td>Can we diagnose the KMT2A leukemia subtype with Raman microscopy?</td>
<td>Patrycja Leszczenko¹, Anna M. Nowakowska², Justyna Jakubowska², Agata Pastorczak²,</td>
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<td>Marta Zabczynska², Wojciech Mlynarski², Malgorzata Baranska¹, Kinga Ostrowska²,</td>
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<td>Katarzyna Majzner¹</td>
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<td>²Department of Pediatric, Oncology and Hematology, Medical University of Lodz</td>
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<td>15:45-15:55</td>
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<td>Pretreatment routines in analysis of Raman spectra recorded in different excitation wavelength and its effect on classification models</td>
<td>Sara Mostafapour¹, Thomas Dörfer², Ralf Henke², Petra Rösch², Jürgen Popp¹, Thomas Bocklitz³</td>
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<td>³Institute of Physical Chemistry and Abbe Centre of Photonics, Friedrich Schiller University of</td>
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<td>Computer Science, Faculty of Mathematics, Physics &amp; Computer Sc</td>
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<td>16:00-16:10</td>
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<td>Infrared molecular fingerprinting for multi-phenotyping of human health and disease</td>
<td>Kepesidis V. Kosmas¹, Marinus Huber², Liudmila Voronina¹, Tarek Eissa¹, Frank Fleischmann¹,</td>
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<td>Cristina Leonardo¹, Jacqueline Hermann¹, Ina Koch³, Thomas Kolben³, Gerald Schulz³, Friedrich</td>
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<td>Jokisch³, Juergen Behr³, Nadia Harbeck³, Maximilian Reiser³, Christian Stief³, Ferenc Krausz³,</td>
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<td>Mihaela Zigman¹</td>
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<td>¹Ludwig Maximilian University of Munich (LMU)</td>
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<td>²Max Planck Institute of Quantum Optics (MPQ)</td>
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<td>³Asklepios Biobank for Lung Diseases, Department of Thoracic Surgery, Member of the German Center</td>
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<td>for Lung Research, DZL, Asklepios Fachkliniken München-Gauting</td>
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<td>⁴University Hospital of the Ludwig Maximilians University Munich (LMU), Department of Obstetrics</td>
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<td>and Gynecology, Breast Center and Comprehensive Cancer Center (CCLMU)</td>
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<td>⁵University Hospital of the Ludwig Maximilians University Munich (LMU), Department of Urology</td>
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<td>⁶University Hospital of the Ludwig Maximilians University Munich (LMU), Department of Internal</td>
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<td>⁷University Hospital of the Ludwig Maximilians University Munich (LMU), Department of Clinical</td>
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<td>15:00-15:10</td>
<td><strong>Nonlinear vibrational spectroscopy</strong></td>
<td>Raman and Stimulated Raman Scattering characterization of carotenoids and amyloid beta deposits in Alzheimer's Disease brain samples</td>
<td>Freek Ariese¹, Benjamin Lochocki², Liron Zada³, Loes Ettema¹, Can Keskin¹, Jinke Van der Sluis¹, Robert W. Schmidt¹ ¹LaserLaB, Vrije Universiteit ²ARCNL</td>
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<td>15:15-15:25</td>
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<td>Glucose and lipid metabolism in endothelium inflammation studied by Raman microscopy</td>
<td>Aleksandra Borek-Dorosz², Anna Pieczara², Jagoda Orleańska³, Krzysztof Brzozowski³, William Tipping⁵, Duncan Graham⁵, Malgorzata Baranska³, Katarzyna Majzner³ ¹Jagiellonian University in Kraków, Faculty of Chemistry, Department of Chemical Physics, 2 Gronostajowa Str., Krakow, Poland ²Jagiellonian University in Kraków, Jagiellonian Centre for Experimental Therapeutics (JCET), 14 Bobrzynskiego Str., Krakow, Poland ³Jagiellonian University in Kraków, Faculty of Chemistry, Department of Chemical Physics, 2 Gronostajowa Str., Krakow, Poland ⁴Jagiellonian University in Kraków, Faculty of Chemistry, Department of Chemical Physics, 2 Gronostajowa Str., Krakow, Poland ⁵Centre for Molecular Nanometrology, WestCHEM, Department of Pure and Applied Chemistry, Technology and Innovation Centre, University of Strathclyde, Glasgow G1 1RD, United Kingdom</td>
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<td>15:30-15:40</td>
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<td>Stimulated Raman scattering imaging – 3D spatial generation</td>
<td>Ronja Eriksson¹, Per Gren¹, Mikael Sjödahl¹, Kerstin Ramser¹ ¹Department of Engineering Sciences and Mathematics, Luleå University of Technology</td>
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<td>15:45-15:55</td>
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<td>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”</td>
<td>Anna Pieczara¹, Aleksandra Borek-Dorosz¹, Szymon Buda¹, William Tipping², Duncan Graham², Robert Pawlowski³, Jacek Młynarski³, Malgorzata Baranska³ ¹Jagiellonian University ²University of Strathclyde ³Polish Academy of Sciences</td>
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<td>16:00-16:10</td>
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<td>Stimulated Raman scattering (SRS) microscopy to investigate pharmaceutical co-crystal formation</td>
<td>Oona Auvinen¹, Alba Arbiol¹, Tom Konings¹, Teemu Tomberg¹, Leena Peltonen¹, Clare Strachan¹, Jukka Saarinen¹ ¹Division of Pharmaceutical Chemistry and Technology, Faculty of Pharmacy, University of Helsinki</td>
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<td>15:00-15:15</td>
<td><strong>Advanced characterization of materials</strong></td>
<td>Inside block copolymer micelles – An AFM-TERS study on the interfacial influences on the core crosslinking efficiency</td>
<td>Christiane Höppener¹, Xinyue Wang², Johanna Elter¹, Felix Schacher¹, Volker Deckert¹ ¹Leibniz Institute of Photonic Technologies (IPHT) ²Institute of Physical Chemistry, Friedrich Schiller University ³Institute of Organic Chemistry and Macromolecular Chemistry, Friedrich Schiller University</td>
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<td>15:20-15:35</td>
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<td>Towards the compactness and permeability of the polymer brushes studied by surface-enhanced Raman spectroscopy</td>
<td>Marek Procházka¹, Monika Spasovová², Markéta Vrabcová², Josef Štěpánek¹, Ondřej Kylián³, Hana Vaisocherová-Lísalová³ ¹Institute of Physics, Faculty of Mathematics and Physics, Charles University ²Department of Optical and Biophysical Systems, Institute of Physics of the Czech Academy of Sciences; Institute of Physics, Faculty of Mathematics and Physics, Charles University ³Department of Macromolecular Physics, Faculty of Mathematics and Physics, Charles University ⁴Department of Optical and Biophysical Systems, Institute of Physics of the Czech Academy of Sciences</td>
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<td>15:40-15:50</td>
<td>Characterisation and evaluation of molecularly imprinted polymers using surface enhanced infrared absorption (SEIRA) spectroscopy.</td>
<td>Armel F. T. Waffo¹, Sagie Katz¹, Giorgio Caserta¹, Aysu Yarman², Bettina Neumann³, Ulla Wollenberger³, Frieder W. Scheller³</td>
<td>¹Technische Universität Berlin  ²Turkish-German University  ³University of Potsdam</td>
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<td>15:55-16:05</td>
<td>Enhancement of the E12g and A1g Raman modes and Layer Identification of 2H-WS2 Nanosheets With Metal Coatings</td>
<td>Bharathi Rajeswaran¹, Rajasheer Konar¹, Gilbert Daniel Nessim², Yaakov Raphael Tischler¹</td>
<td>¹Bar-Ilan University, Israel  ²Bar-Ilan University, Ramat Gan, Israel</td>
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<tr>
<td>A0-03</td>
<td>(G) Analytical applications</td>
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<td>Chair: Maria-Paula Marques</td>
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<td>15:00-15:15</td>
<td>Insights into forensic analysis of peripheral blood stains on natural and synthetic fabrics using ATR-FTIR spectroscopy</td>
<td>Entesar Al-Hetlani¹, Zainab Husain¹, Mohamed Amin¹</td>
<td>¹Kuwait University</td>
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<td>15:20-15:35</td>
<td>Revealing the Secrets of Graeco-Roman Egyptian Mummies Using Vibrational Spectroscopic Techniques</td>
<td>Bayden Wood¹, Callum Gassner¹, Magdalena Giergiel¹, Ankit Dodla¹, Janet Davey²</td>
<td>¹Monash University  ²Victoria Institute of Forensic Medicine</td>
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<td>15:40-15:50</td>
<td>Fingermark analysis utilizing ATR-FTIR spectroscopy for forensic discrimination of smoker and nonsmoker</td>
<td>Mohamed O. Amin¹, Entesar Al-Hetlani¹, Igor K. Lednev Lednev²</td>
<td>¹Kuwait University  ²University at Albany</td>
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<td>15:55-16:05</td>
<td>Deep UV Raman spectroscopy for post-mortem interval determination</td>
<td>Anna Wójtowicz¹, Luis Perez Almodovar², Igor K. Lednev², Renata Wietecha-Postuszny³</td>
<td>¹Laboratory for Forensic Chemistry, Department of Analytical Chemistry, Jagiellonian University  ²Department of Chemistry, University at Albany, SUNY</td>
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<td>A0-01</td>
<td>(H) Biodiagnostic spectroscopy</td>
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<td>Chair: Hugh Byrne</td>
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<td>15:00-15:10</td>
<td>Raman-based evaluation of in vitro myeloid precursor differentiation toward macrophages</td>
<td>Adriana Adamczyk¹, Anna Nowakowska¹, Justyna Jakubowska², Katarzyna Majzner³, Małgorzata Baranska¹</td>
<td>¹Jagiellonian University in Krakow, Faculty of Chemistry, Department of Chemical Physics, Kraków, Poland  ²Department of Pediatrics, Oncology and Hematology, Medical University of Lodz, Łódz, Poland</td>
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<td>15:15-15:25</td>
<td>Brillouin and Raman micro-spectroscopy to characterise human bone and cartilage: from healthy phenotype to biomedical applications in osteoarthritis and bone infections.</td>
<td>Martina Alunni Cardinali¹, Sara Stefani¹, Marco Govoni², Dante Dallari², Leonardo Vivarelli², Matilde Tschon³, Silvia Brogini³, Alessandra Maso⁴, Elisa Storni³, Francesca Valentì⁵, Melania Maglio⁶, Maurizio Mattarelli⁶, Alessandra Anna Passeri⁶, Silvia Caponi⁷, Assunta Morresi¹, Paolo Sassi¹, Daniele Fioretto⁶</td>
<td>¹Dep. Chemistry, Biology and Biotechnology, University of Perugia  ²Reconstructive Orthopaedic Surgery and Innovative Techniques – Musculoskeletal Tissue Bank, IRCCS Istituto Ortopedico Rizzoli  ³Surgical Sciences and Technologies, IRCCS Istituto Ortopedico Rizzoli  ⁴Laboratory of Microbiology and GMP Quality Control, IRCCS Istituto Ortopedico Rizzoli  ⁵Dep. of Pharmacy and Biotechnology, University of Bologna  ⁶Dep. Physics and Geology, University of Perugia  ⁷CNR- Dep. Physics and Geology</td>
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<td>15:30-15:40</td>
<td>Fourier Transform Infrared Microspectroscopy identifies single cancer cells in blood. A feasibility study towards liquid biopsy. Lewis M. Dowling¹, Paul Roach², Eirik A. Magnussen³, Achim Kohler³, Srinivas Pillai⁴, Daniel G. Van Pittius⁵, Ibraheem Yousef⁶, Josep Sulé-Suso⁷ ¹Keele University ²Loughborough University ³Norwegian University of Life Sciences ⁴University Hospitals of North Midlands ⁵ALBA Synchrotron Light Source</td>
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<td>15:45-15:55</td>
<td>Raman spectroscopy in the biochemical characterisation of THP-1 leukemic cells modified to overexpress mutated FLT3 receptor. Sylwia Orzechowska¹, Paulina Laskowska², Aleksandra Borek-Dorosz¹, Anna Maria Nowakowska¹, Wiktoria Korona¹, Marcin Szydłowski¹, M. Zasowska², Piotr Juszczyński², Małgorzata Barańska³, Piotr Mrówka¹, Katarzyna Majzner¹ ¹Jagiellonian University, Faculty of Chemistry ²Department of Experimental Hematology, Institute of Hematology and Transfusion Medicine ³Jagiellonian University, Faculty of Chemistry; Jagiellonian Centre for Experimental Therapeutics (JCET), Jagiellonian University ⁴Department of Experimental Hematology, Institute of Hematology and Transfusion Medicine; Department of Biophysics, Physiology and Pathophysiology, Medical University of Warsaw</td>
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<td>16:00-16:10</td>
<td>Identification of Chemical Modifications of Myocardium in Heart-Failure with Preserved Ejection Fraction Leonardo Pioppi¹, Reza Parvan², Alan Samrend², Gustavo Jose Justo Da Silva², Marco Paolantoni¹, Alessandro Cataliotti², Paola Sassi¹ ¹Department of Chemistry, Biology and Biotechnology, University of Perugia ²Institute for Experimental Medical Research, Oslo University Hospital and University of Oslo</td>
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<td>16:30-18:45</td>
<td>POSTER SESSION 3: Topics G, H, I Chairs: Sara Miller, Christian Johannessen</td>
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<td>16:30-17:30</td>
<td>A0-01 Flash Presentations</td>
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| 17:30-18:45  | Poster Session  

Thursday

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<th>Time</th>
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| 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 Gierlinger¹ ¹University 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 Mosig¹ ¹Ruhr University Bochum, Center for Protein Diagnostics  |
| 10:15-10:45  | Coffee Break  |
| 10:45-12:10  | SESSION 1  |
| 10:45-10:55  | 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 Chalmers¹, Sara Miller¹, Teemu Tomberg², Keith Gordon¹ ¹Te Whai Ao – The Dodd-Walls Centre for Photonic and Quantum Technologies and Department of Chemistry, University of Otago ²Division 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. Kalka¹, Andrzej M. Turek¹ ¹Jagiellonian 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 Broggio1, Andrea Masella1, Giulia De Poli1, Manuela Bazzarelli1, Dario Polli2, Matteo Bregonzio1, Renzo Vanna2
1Datrix S.p.A.
2Department of Physics, Politecnico di Milano / Istituto di Fotonica e Nanotecnologie (IFN), Consiglio Nazionale delle Ricerche (CNR)
3Istituto di Fotonica e Nanotecnologie (IFN), Consiglio Nazionale delle Ricerche (CNR)

11:30-11:40 Tensor decomposition assisted super-resolution in polarized Raman microscopy
Andrii Kutsyk1, Oleksii Ilichenko1, Yurii Pilhun2, Jens Wenzel Andreasen1
1Technical University of Denmark
2Lightnovo ApS

11:45-11:55 Extensive Evaluation of Machine Learning Models and Data Preprocessings for Raman Modeling in Bioprocessing
Michaela Poth1, Gordon Magill2, Alois Filgertshofer3, Oliver Popp1, Tobias Großkopf1
1Therapeutic Modalities, Roche Innovation Center Munich, Bioprocess Research, Roche Pharma Research and Early Development
2Cell Culture Development and Bioprocess, Genentech Inc.

11:55-12:05 Charge Transfer Across Hydrophobic Interfaces
Saranya Pullanchery1, Sergey Kulik1, Benjamin Rehl1, Ali Hassanali2, Sylvie Roke1
1Laboratory for Fundamental BioPhotonics, Institute of Bioenginering (IBI), School of Engineering (STI), École Polytechnique Fédérale de Lausanne (EPFL)
2The Abdus Salam International Centre for Theoretical Physics
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<th>Time</th>
<th>Session A0-04: Advanced characterization of materials</th>
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<td>10:45-10:55</td>
<td>Ibuprofen/chitosan matrices as a promising base for intestinal soft capsules</td>
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<td>Barbara Gieroba¹, Maryna Khalavka², Olena Mozgova³, Paulina Kazimierczak⁴, Grzegorz Kalisz¹, Izabela S. Pięta¹, Liudmyla Nosach¹, Vladyslav Vivcharenko⁴, Agata Przekora¹, Anna Sroka-Bartnicka¹</td>
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<td>¹Independent Unit of Spectroscopy and Chemical Imaging, Faculty of Biomedical Sciences, Medical University of Lublin, Chodzki 4a, 20-093 Lublin, Poland</td>
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<td>²Independent 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, Pushkinska 63 St., 6100</td>
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<td>³Independent 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, Valentinivska 4 St., 6</td>
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<td>⁴Independent Unit of Tissue Engineering and Regenerative Medicine, Faculty of Biomedical Sciences, Medical University of Lublin, Chodzki 1, 20-093 Lublin, Poland</td>
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<td>⁵Institute of Physical Chemistry Polish Academy of Sciences, Kasprzaka 44/52, 01-224 Warsaw, Poland</td>
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<td>⁶Independent 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 Chemistry</td>
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<td>11:00-11:10</td>
<td>Low frequency Raman spectroscopy for characterization of amorphous and crystalline variably substituted hydroxyapatites</td>
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<td>Joshua Kirkham¹, Tim Kortner², Kārlis Bērziņš¹, Cushla McGoverin³, Keith Gordon¹, Sara Miller¹</td>
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<td>¹Te Whai Ao – The Dodd-Walls Centre for Photonic and Quantum Technologies and Department of Chemistry, University of Otago</td>
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<td>²Department of Chemistry, Syracuse University, Center for Science and Technology</td>
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<td>³Te Whai Ao – The Dodd-Walls Centre for Photonic and Quantum Technologies, and Department of Physics, University of Auckland</td>
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<td>11:15-11:25</td>
<td>Exploring the glycosaminoglycan structure: does it fold and how?</td>
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<td>Gergo Peter Szekeres¹, Jan Horlebein², Jerome Riedel¹, Gert Von Helden², Mark Mero³, Kevin Pagel¹, Zsuzsanna Heiner¹</td>
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<td>¹Freie Universität Berlin, Fritz-Haber-Institut der Max-Planck-Gesellschaft</td>
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<td>²Fritz-Haber-Institut der Max-Planck-Gesellschaft</td>
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<td>³Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy</td>
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<td>⁴School of Analytical Sciences Adlershof, Humboldt-Universität zu Berlin</td>
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<td>11:30-11:40</td>
<td>Phosphine Halogen-Bonded Complexes: Investigated Using Matrix Isolation IR Spectroscopy</td>
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<td>Elliot Tay¹, Corentin Grassin¹, Clemens Müller¹, Christian Merten¹</td>
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<td>¹Organische Chemie II, Fakultät für Chemie und Biochemie</td>
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<td>11:45-11:55</td>
<td>Raman spectroscopy for investigation of interaction within polymer based magnetic multicomponent scaffolds</td>
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<td>Anna Kołodziej¹, Małgorzata Świętek², Anna Hlukhaniuk², Daniel Horák², Aleksandra Wesełucha-Birczyńska¹</td>
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<td>¹Faculty of Chemistry, Jagiellonian University</td>
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<td>²Institute of Macromolecular Chemistry, Czech Academy of Sciences</td>
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<td>12:00-12:10</td>
<td>Which method will distinguish nanofibrous carbon materials?</td>
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<td>Aleksandra Wesełucha-Birczyńska¹, Maria Pajda², Elżbieta Dluгоň³, Krzysztof Morajka¹, Marek Michał¹, Marta Błażewicz⁴</td>
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<td>⁴AGH – University of Science and Technology, Faculty of Materials Science and Ceramics, AGH – University of Science and Technology, Faculty of Materials Science and Ceramics</td>
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<td>A0-03</td>
<td>(D) Spectroscopy of surface&amp;interfaces</td>
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<td>10:45-11:00</td>
<td>Surface-enhanced resonance Raman spectro-electrochemistry as a tool to study redox-related structural changes in (bio)chemistry in-situ</td>
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<td>Michelle Mahler¹, Patrycja Kielb¹</td>
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<td>¹University of Bonn</td>
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<td>11:05-11:20</td>
<td>Tip-enhanced Raman spectroscopy for nanoscale studying of catalytic. systems</td>
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<td>Bin Ren¹, Xiang Wang¹, Tengxiang Huang¹, Huishu Feng¹</td>
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<tr>
<td>11:25-11:35</td>
<td>Mechanistic insights of conjugated acetylenic polymers for the photoelectrochemical nitrogen</td>
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<td>reduction reaction to ammonia</td>
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<td>11:40-11:50</td>
<td>Revealing the Size Effect of Pd/Au Bimetallic Catalysts at Nanoscale with Tip-enhanced Raman</td>
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<td>Spectroscopy</td>
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<td>11:55-12:05</td>
<td>The study of correlated Stokes-and-anti-Stokes in normal Raman and in Surface-Enhanced</td>
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<td>Raman Scattering (SERS)</td>
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<tr>
<td>A0-01</td>
<td>(H) Biodiagnostic spectroscopy</td>
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<td>10:45-11:00</td>
<td>Raman imaging and AFM studies of human colon tissues and cells – cholesterol impact on CRC</td>
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<td>development</td>
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<tr>
<td>11:05-11:20</td>
<td>Raman Spectroscopy for Pre-Disease Analysis</td>
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<td>11:25-11:35</td>
<td>Application of Raman spectroscopy to examine tattoo pigments in tissues</td>
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<td>11:40-11:50</td>
<td>Raman analysis of breast microcalcifications, correlation with pathology</td>
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<td>11:55-12:05</td>
<td>Pre-clinical characterization of Osteopetrosis in Mice Models by Raman microscopy</td>
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<td>12:10-13:10</td>
<td>Lunch</td>
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<tr>
<td>13:10-14:30</td>
<td>SESSION 2</td>
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<tr>
<td>A1-01</td>
<td>(I) Chemometrics &amp; machine learning</td>
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<tr>
<td>13:10-13:20</td>
<td>Long short-term memory and Transformer in Classification and Correction of ATR distorted</td>
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<td>spectrum</td>
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<tr>
<td>13:40-13:50</td>
<td>Characterization of root tissue development associated with lodging tendency in tef using Raman micro-spectroscopyscopy</td>
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<tr>
<td>13:55-14:05</td>
<td>Plasmonic surface enhanced infrared spectroscopy aided with artificial intelligence for structural protein biomarker based neurodegenerative disease detection</td>
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<tr>
<td>14:10-14:20</td>
<td>The use of NIR spectroscopy for the analysis of Fumonisin B1 (FB1)</td>
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<tr>
<td>14:25-14:35</td>
<td>A multivariate surface-enhanced infrared absorption (SEIRA) method based on quantum dots and universal attenuated total reflectance (UATR) asssor for atrazine determination</td>
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<tr>
<td>A1-02</td>
<td>(J) Computational approaches</td>
</tr>
<tr>
<td>13:10-13:25</td>
<td>Raman Optical Activity: Simulations Outside and In Resonance</td>
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<tr>
<td>13:30-13:45</td>
<td>CHIROPTICAL SPECTRA: WHEN CALCULATIONS MEET THE EXPERIMENT</td>
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<td>13:50-14:00</td>
<td>A study of synchrotron-based UV-resonance Raman spectra of N-acetylamino saccharides – In combination with their ATR-far ultraviolet spectroscopy study</td>
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<td>14:05-14:15</td>
<td>Vibrational Circular Dichroism of Chiral Crystals: The Interplay of Symmetry and Chirality</td>
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<td>14:35-14:45</td>
<td>Quantitative evaluation of IR and corresponding VCD spectra</td>
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<tr>
<td>A0-04</td>
<td>(A) Advanced characterization of materials</td>
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<tr>
<td>13:10-13:20</td>
<td>Raman Confocal Imaging for materials at high temperatures</td>
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<td>13:25-13:35</td>
<td>Automated Quantitative Analysis of (Microplastic) Particles and Fibers down to 1 µm by Raman Microspectroscopy</td>
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<td>13:40-13:50</td>
<td>Investigating Degradation of Poly(vinyl chloride) by Spectroscopic Methods</td>
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<td>14:10-14:20</td>
<td>Imaging of Three-dimensional Molecular Orientation Using FT-IR, Raman, and O-PTIR Microspectroscopies of various samples</td>
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<tr>
<td>A0-03</td>
<td>(D) Spectroscopy of surface/interfaces</td>
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<tr>
<td>13:10-13:25</td>
<td>Quantifying Large-Scale Structural Changes During pH-Induced Channel Opening of Influenza A M2 using Surface-enhanced Infrared Absorption Spectroscopy</td>
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<td>13:30-13:45</td>
<td>Mechanistic insights into the electrosynthesis of chemical feedstocks by in situ Raman and ATR-FTIR spectro-electrochemistry</td>
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<td>13:50-14:00</td>
<td>Nanoscale hyperspectral imaging of biologically relevant molecules</td>
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<td>14:05-14:15</td>
<td>Nanospectroscopy imaging of the molecule/metal interaction</td>
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<td>A0-01</td>
<td>(H) Biodiagnostic spectroscopy</td>
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<td>13:10-13:20</td>
<td>Study on the effects of cryoconservation on human platelets</td>
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<td>13:25-13:35</td>
<td>Fighting peripheral nervous system tumors-hyperspectral imaging as a novel approach to monitor the therapeutic efficacy of cannabidiol</td>
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<td>13:40-13:50</td>
<td>Infrared tissue analysis of Hirschsprung’s disease</td>
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<td>13:55-14:05</td>
<td>Infrared spectral biomarkers of neurodegenerative diseases</td>
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<td>Lila Lovergne¹, Dhruba Ghosh², Renaud Schuck¹, Aris Polyzos¹, Michael Martin², Edward Barnard⁴,</td>
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<td>James Brown³, Cynthia McMurray⁴</td>
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<td>¹Lawrence Berkeley National Laboratory/ Division of Molecular Biophysics and Integrated Bioimaging</td>
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<td>²Lawrence Berkeley National Laboratory/ Department of Statistics</td>
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<td>³Lawrence Berkeley National Laboratory/ Advanced Light Source</td>
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<td>⁴Lawrence Berkeley National Laboratory/ Molecular Foundry</td>
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<td>⁵Lawrence Berkeley National Laboratory/ Department of Statistics, and Division of Environmental Genomics and Systems Biology</td>
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<td>14:10-14:20</td>
<td>Multimodal spectroscopic imaging of cervical cancer cells exposed to the adaptogenic drug</td>
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<td>Ewa Pięta¹, Katarzyna Pogoda¹, Klaudzia Suchy¹, Karolina Chrabąszcz², Czesława Paluszkiewicz¹,</td>
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<td>Wojciech Kwiatek¹</td>
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<td>¹Institute of Nuclear Physics Polish Academy of Sciences</td>
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<td>14:25-14:35</td>
<td>FTIR imaging of kidney tissues to diagnose hypertensive organ damage and pharmacological treatment</td>
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<td>Paola Sassi¹, Leonardo Pioppi¹, Niki Tombolesi¹, Reza Parvan², Gustavo Da Silva², Raffaele Altara³,</td>
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<td>Marco Paolantoni¹, Assunta Morresi¹, Alessandro Cataliotti²</td>
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<td>¹University of Perugia</td>
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<td>³Maastricht University</td>
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<td>14:45-15:00</td>
<td>SHIM-POL presentation Titel: Nice to have two features in one – the new AIRsight</td>
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<td>Subject: First measurement results obtained with the new AIRsight. The unique FTIR and</td>
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<td>Raman Microscope.</td>
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<td>18:30</td>
<td>Conference Dinner</td>
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<td>Friday</td>
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<td>9:00-10:15</td>
<td>Plenary Session</td>
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<td>Chair: Alexandre Brolo</td>
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<td>9:00-9:30</td>
<td>Molecular Optomechanics Approach to Surface-Enhanced Raman Scattering</td>
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<td>Javier Aizpurua¹</td>
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<td>¹Center for Materials Physics (CSIC-UPV/EHU)</td>
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<td>Chair: Katarzyna Marzec</td>
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<td>9:40-10:10</td>
<td>Increasing the utility of infrared spectroscopic imaging by high performance instrumentation</td>
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<td>Rohit Bhargava¹</td>
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<td>¹Departments of Bioengineering, Electrical &amp; Computer Engineering, Mechanical Science &amp;</td>
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<td>Engineering, Chemical and Biomolecular Engineering, and Chemistry, Beckman Institute for</td>
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<td>Advanced Science and Technology, Cancer Center at Illinois, University of Illinois at Urbana-</td>
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<td>Champaign, 405 N. Mathews Ave., Urbana, IL 61801 USA</td>
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<td>10:15-10:45</td>
<td>Coffee Break</td>
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<td>10:45-12:10</td>
<td>SESSION 1</td>
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<td>(1) Chemometrics&amp;machine learning</td>
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<td>Chair: Milda Pucetaite</td>
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<td>10:45-11:00</td>
<td>In silico experimentation to guide optimization and experimental design in clinical spectroscopy.</td>
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<td>David Perez-Guaita¹, Victor Navarro-Esteve¹, Jaume Bejar-Grimalt¹, Angel Sanchez-Illana¹,</td>
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<td>Hugh J. Byrne²</td>
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<td>²Technological University Dublin</td>
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<td>11:05-11:20</td>
<td>Sparse Wavelength Sampling in Mid-Infrared Spectroscopy</td>
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<td>Valeria Tafintseva¹, Miriam Aledda¹, Boris Zimmermann¹, Nagesvar Patel¹, Volha Shapaval¹,</td>
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<td>Achim Kohler¹</td>
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<td>¹Norwegian University of Life Sciences</td>
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<td>11:25-11:35</td>
<td>Green Pharmaceutical Quality Control via Infrared Spectroscopy</td>
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<td>Silke Lehner¹, Mona Tawab², Holger Latsch², Sandra Ganß², Boris Mizaikoff³, Robert Stach¹</td>
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| 11:40-11:50| Influence of Infrared Imaging measurement modes on breast tissue recognition and cancer diagnosis | Danuta Liberda¹, Tomasz P. Wróbel²  
¹Jagiellonian University, Doctoral School of Exact and Natural Sciences, Prof. St. Łojasiewicza 11, PL30348, Cracow, Poland  
²Solaris 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 Magnussen¹, Boris Zimmermann², Uladzislau Blazhko², Simona Dzurendova², Benjamin Dupuy-Galet³, Dana Byrtusova³, Florian Muthreich³, Valeria Tafintseva³, Kristian Hovde Liland³, Volha Shapaval³, Achim Kohler³  
¹Norwegian University of Life Sciences  
²University 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 Cheeseman¹  
¹Gaussian, 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 Bogaerts¹, James Cheeseman¹, Wouter Herrebout¹, Christian Johannessen¹  
¹University of Antwerp  
²Gaussian Inc. |
| 11:15-11:25| Simulation of vibrational spectroscopies in various environments         | Vincent Liegeois¹  
¹NISM, Unamur |
| 11:30-11:40| Anharmonicity of amide bands in NIR region – overtones, combinations, structural fingerprint of peptides | Justyna Grabska¹, Krzysztof B. Bec¹, Christian W. Huck¹  
¹University of Innsbruck |
| 11:45-11:55| Resonance Raman Optical Activity: how to properly measure, correct and simulate spectra | Grzegorz Zajać¹, Ewa Machalska², Katarzyna Pajor³, Josef Kapitán³, Petr Bouri³, Małgorzata Baranska⁶  
¹Jagiellonian Centre for Experimental Therapeutics (JCET), Jagiellonian University  
²Jagiellonian Centre for Experimental Therapeutics (JCET), Jagiellonian University; Institute of Nuclear Chemistry and Technology  
³Faculty of Chemistry, Jagiellonian University  
⁴Department of Optics, Palacký University Olomouc  
⁵Institute of Organic Chemistry and Biochemistry, Academy of Sciences  
⁶Faculty 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 Daturi¹  
¹Laboratory 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-Paczkowska¹  
¹Faculty 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 Bracco¹, Helios Vocca¹, Silvia Corezzi², Alessandro Di Michele², Laura Silenzi³, Angela Trapananti³, Flavio Travasso³, Stefano Colace³, Michele Magnozzi³, Paola Sassi³  
¹Department of Chemistry, Biology and Biotechnology, University of Perugia and Istituto Nazionale di Fisica Nucleare, Sezione di Perugia  
²School of Science and Technology – Physics Division, University of Camerino and Istituto Nazionale di Fisica Nucleare, Sezione di Perugia  
³Department of Physics, Università di Genova |

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**Notes:**
- All times are in 24-hour format.
- Authors' affiliations are listed at the end of each entry.
- Some affiliations include multiple institutions, which are separated by semicolons.
- The table structure is maintained to reflect the organization of the schedule.
- The final entries indicate the scope and contributors of the research topics.
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<th>Time</th>
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<tr>
<td>11:40-11:50</td>
<td>Can elevated temperatures in HTGR nuclear reactors reverse irradiation damage in graphite? – high-temperature in-situ Raman spectroscopy study</td>
<td>Magdalena Gawęda¹, Piotr Jeleń², Łukasz Kurpaska³, Jacek Jagielski³ ¹NOMATEN CoE, NOMATEN MAB, National Centre for Nuclear Research ²AGH University of Science and Technology ³National Centre for Nuclear Research, Łukasiewicz Institute for Microelectronics &amp; Photonics</td>
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<td>10:45-11:00</td>
<td>Surface-enhanced Raman Scattering in scaffolds for 3D cell cultures</td>
<td>Judith Langer¹, Javier Plou², Clara Clara García-Astrain³, Beatriz Molina-Martínez³, Luis M. Láz-Marzán⁴ 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) (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</td>
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<td>11:05-11:15</td>
<td>Spectroscopic study of extracellular vesicles using plasmonic nanoobjects</td>
<td>Timea Bebesi¹, Marcell Pálmai¹, Anikó Gaál¹, Imola Csilla Szigyarto¹, Orsolya Bálint-Hakkel², Zoltán Varga¹, Judith Mihály¹ ¹Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences ²Institute of Technical Physics and Material Sciences, Centre for Energy Research</td>
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<td>11:20-11:30</td>
<td>Giant plasma membrane vesicles as the model systems to resolve nanoscale heterogeneity of native lipid membranes</td>
<td>Katarzyna Pogoda¹, Klemencja Berghauzen-Maciejewska², Natalia Piergies², Karolina Chrabąszcz², Czesława Paluszkiewicz², Wojciech Kwiatek² ¹Institute of Nuclear Physics Polish Academy of Sciences ²Institute of Nuclear Physics PAN</td>
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<td>11:35-11:45</td>
<td>SERS based detection of cytosine methylation in genomic DNA</td>
<td>Stefania D. Iancu¹, Vlad Moisoiu¹, Adrian B. Tigu², Andrei Stefanu¹, Zoltán Bálint¹, Ciprian Tomuleasa², Nicolae Leopold¹ ¹Faculty of Physics, Babeș-Bolyai University ²Medfuture Research Center for Advanced Medicine, Iuliu Hatieganu University of Medicine and Pharmacy</td>
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<tr>
<td>11:05-11:15</td>
<td>SERS analysis of urine for prostate cancer detection</td>
<td>Nicolae Leopold², Stefania D. Iancu¹, Andrei Stefanu¹, Vlad Moisoiu¹, Teodora Telecan², Iulia Andras², Nicolae Crisan² ¹Faculty of Physics, Babeș-Bolyai University ²Urology Department, Iuliu Hatieganu University of Medicine and Pharmacy</td>
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<tr>
<td>11:20-11:30</td>
<td>Vibrational spectroscopy for differential diagnosis of patients with rheumatoid and psoriatic arthritis</td>
<td>Sylwester Mazurek¹, Izabela Kokot², Agnieszka Piwowar², Renata Sokolik², Monika Kacperczyk², Kamil Rodak², Roman Szostak¹, Lucyna Korman², Ewa Kratz² ¹University of Wroclaw, Department of Chemistry ²Wroclaw Medical University</td>
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<td>11:35-11:45</td>
<td>Infrared spectroscopy for rapid and objective diagnosis of the etiology of infection as bacterial or viral using a simple peripheral blood test. Ahmad Salman¹, Uraib Sharaha², Guy Beck³, Yotam D. Eshel⁴, Gal Cohen-Logasi⁴, Adam H. Agbaria⁵, Itshak Lapidoṭ⁶, Joesh Kapelushnik⁶, Mahmoud Huleihel⁶, Shaul Mordechai⁶</td>
<td>SCE-Sami Shamoon College of Engineering/Department of Physics</td>
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1SCE-Sami Shamoon College of Engineering/Department of Physics  
2Ben-Gurion University/Department of Microbiology, Immunology, and Genetics  
3Soroka University Medical Center/Department of Hematology and Oncology, Saban Pediatric Medical Center  
4SCE-Sami Shamoon College of Engineering/Department of Green Engineering  
5Ben-Gurion University, Department of Physics  
6Afeka Tel-Aviv Academic College of Engineering, Department of Electrical and Electronics Engineering

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Conference Proceedings

Participants are cordially invited to submit a full-length manuscript for publication in a virtual special issue of Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy (SAA), which will be devoted to the 12th International Conference on Vibrational Spectroscopy. Guest editor of the VSI:ICAVS12 will be Prof. Kamilla Malek. Submission is open from August 1, 2023 till December, 31, 2023.

SAA (IF= 4.4) is an interdisciplinary journal that spans from basic to applied aspects of optical spectroscopy in chemistry, medicine, biology, and materials science. The journal publishes original scientific papers that feature high-quality spectroscopic data and analysis.

From the broad range of optical spectroscopies, the emphasis is on electronic, vibrational, or rotational spectra of molecules, rather than on spectroscopy based on magnetic moments.

Topics of particular interest of SAA include, but are not limited to:

- Spectroscopy and dynamics of bioanalytical, biomedical, environmental, and atmospheric sciences,
- Novel experimental techniques or instrumentation for molecular spectroscopy,
- Novel theoretical and computational methods,
- Novel applications in photochemistry and photobiology,
- Novel interpretational approaches as well as advances in data analysis based on electronic or vibrational spectroscopy.
Pre-Conference Workshops

WITec Raman Workshop

Company: Oxford Instruments WITec

New Perspectives in 3D Raman Imaging and Correlative Techniques

3D confocal Raman imaging is a powerful, versatile and increasingly common microscopy technique, capable of quickly identifying the molecules in a sample and visualizing their physical distribution. Correlative microscopy is a hybrid approach that looks at a sample with different microscope technologies, each optimized individually then later linked for a far more detailed analysis of chemical and structural features. This seminar will introduce the fundamental principles of Raman imaging, detail the associated hardware and software, describe several of its variations and provide relevant application examples. Speakers will then highlight the advantages of the Raman imaging providing insights to the latest research trends and technologies.

Workshop Program – room A0-03

13:15-13:30 Registration

13:30-13:40 Welcome

13:40-13:40 New Perspectives in 3D Raman Imaging and Correlative Techniques – Ievgeniia Iermak, Oxford WITec, Ulm, Germany

14:10-14:40 Diverse faces of adipose tissue: what can we learn from Raman-based techniques? – Prof. Agnieszka Kaczor, Jagiellonian University Krakow, Poland

14:40-15:10 Raman Bioimaging of Photosynthetic Microorganisms: New Opportunities and Challenges for Correlative Techniques – Dr. Peter Mojzeš, Charles University, Prague, Czech Republic

15:10-15:25 New Tools and Accessories for Cutting-edge Raman Imaging Results – Ievgeniia Iermak, Oxford WITec, Ulm, Germany

15:25-15:30 Wrap-up

O-PTIR workshop

Company: Photothermal Spectroscopy Corporation (PSC)

Submicron IR and Simultaneous Raman Microscopy with Co-Located Fluorescence Imaging

Part One: 12:00-13:30 (Solaris Synchrotron)

The workshop will start off with live in-person demonstration of the mIRage-LS multimodal IR microscope at the nearby Solaris Synchrotron, hosted by Asst Prof Tomek Wrobel (IR beamline)

Please indicate your intention to join us for this during the registration process as space is limited.

Part Two: 13:30-15:30 (room A0-04, Faculty of Chemistry, Jagiellonian University)

The workshop will feature 3 leading academic guest speakers, all presenting their most recent exciting research and experiences with their O-PTIR systems with an opening introductory talk by Dr. Mustafa Kansiz.

Raman imaging

Company: HORIBA & COMEF Sp. z o.o. Sp. k.

Raman imaging: discover the easiest and the most accurate ways to characterize micro & nanoplastics.

Combine its full power to all your microscope in your lab with correlative microscopy.
Micro and nanoplastics represent one of the biggest challenges facing our societies today, as well as our analytical laboratories. In addition to their apparently massive presence in the environment, their probable harmful consequences for human health make them focused by news standards and regulations which require their detection, identification, and precise quantification.

Join our workshop and discover in live how, with Horiba last born µRaman (LabRAM Soleil) and its Particles-FinderTM software, particles and thus micro and nanoplastics analysis is now accurate and easy to access. Moreover, far to stay limited in only one analytical and imaging technic, discover also during our live demonstration NanoGPS suite, our exclusive solution for quick and easy collocation from one microscope to another. Correlative microscopy has never been so easy!.

**Workshop program – room A0-01**

11:15-11:30 – Registration & welcome

11:30-12:15 – *Micro&Nanoplastic: Latest news about norms and regulation. Discover the HORIBA approach to master the Micro&Nanoplastic analysis* – Dr. Massimiliano Rocchia; Horiba France

12:15-12:35 – *LIVE DEMONSTRATION – NanoGPS Suite: Correlative microscopy solution; switching between microscopes has never been so fast and accurate* – Jocelyne MARCIANO; Horiba France

12:35-12:55 – *LIVE DEMONSTRATION: ParticleFinderTM: fast, accurate and easy particles or microplastics sorting and characterization* – Jocelyne MARCIANO; Horiba France

12:55-13:15 – free exchange, question & answer around the workshop activities and presentations.

DO NOT HESITATE TO BRING YOUR SAMPLE TO OUR BOOTH. DURING ALL THE CONFERENCE... AND COME BACK TO YOUR LAB WITH HIGH ACCURATE RESULTS THANK TO OUR LABRAM SOLEIL
# Awards for the Best Poster and Flash Presentations

| Award for poster presentation | Award for excellence in poster presentation – a $500 award founded by Biointerphases |
| Awards for poster presentation | Two Francis Dunstan Awards for the best posters – £250 founded by Infrared and Raman Discussion Group (IRDG) |
| Awards for Flash Presentations | Three Awards for the best flash presentations - $300 founded by Spectrochimica Acta, Part A: Molecular and Biomolecular Spectroscopy (SAA), Elsevier |
| Award for flash presentations | Audience Award – a tablet founded by Renishaw |
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