



# ICAVS12

12<sup>th</sup> International Conference  
on Advanced Vibrational Spectroscopy

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**27.08-01.09.2023, Krakow, Poland**



CONFERENCE CATALOGUE

# WELCOME

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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# I General Information



# Organizers



JAGIELLONIAN UNIVERSITY  
IN KRAKÓW

Jagiellonian University  
in Krakow



Raman Imaging Group  
Faculty of Chemistry



CLIRSPEC

The International Society  
for Clinical Spectroscopy



Targi  
w Krakowie

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# 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)

Malgorzata 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

Malgorzata Baranska

Katarzyna Majzner

Anna Antolak

Aleksandra Borek-Dorosz

Jakub Dybas

Anna Nowakowska

Ewa Machalska

Sylwia Orzechowska

Szymon Tott

Adrianna Wiśłocka-Orłowska

Grzegorz Zajac

## CLIRSPEC Representatives

Hugh Byrne ..... Ireland

Alex Henderson.....UK

# Jagiellonian University in Kraków



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 Wojtyła, the future Pope John Paul II, were world-famous scholars, and Karol Olszewski and Zygmunt Wroblewski liquified 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.



Collegium Maius assembly hall. Source: JU Centre for Communications and Marketing

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.

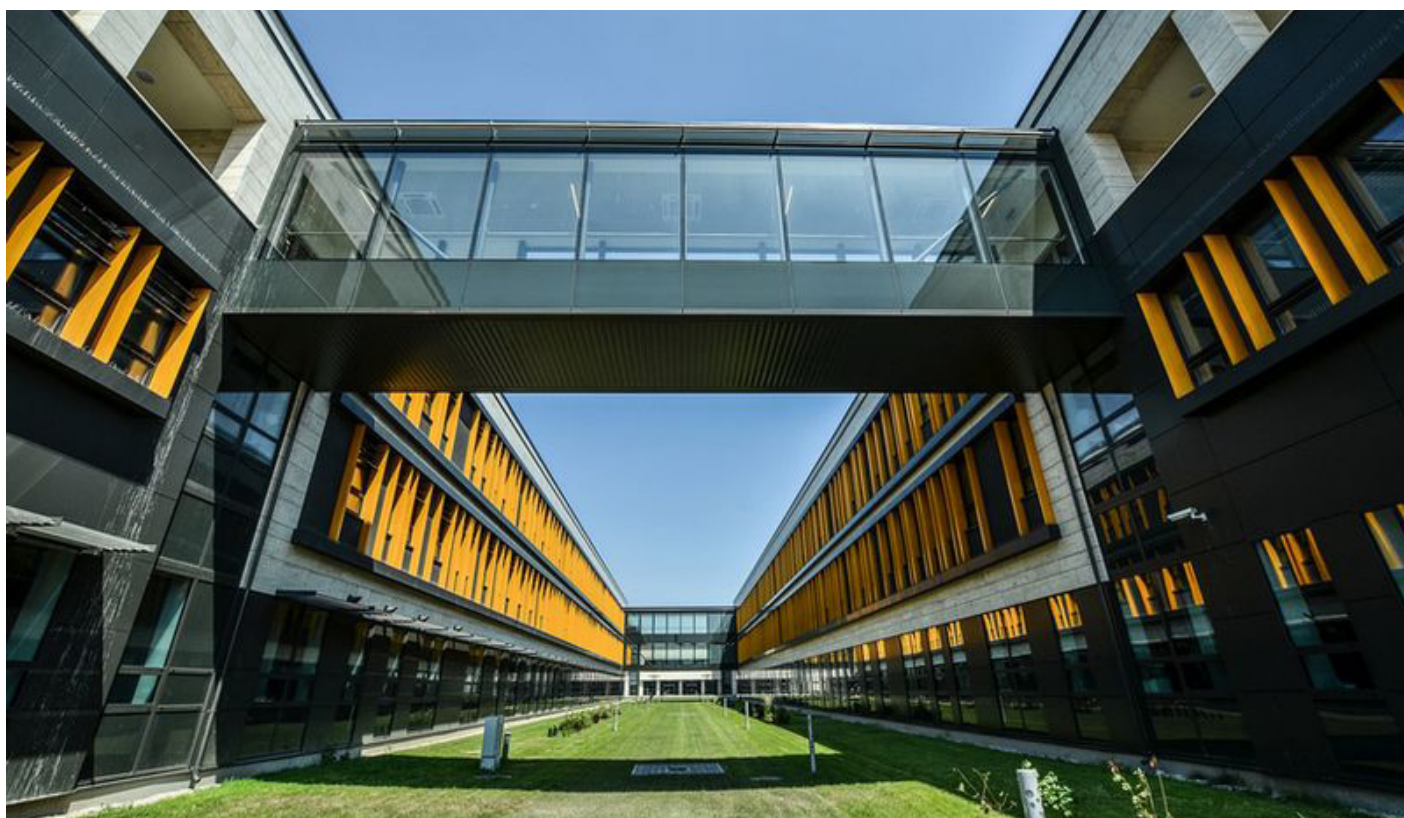




# Faculty of Chemistry

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.  
Galicyjska Street 9  
31-586 Krakow  
<http://kongresy.krakow.pl>  
Phone: +48 12 651 90 71, +48 12 651 95 42  
Email: [icavs2023@targi.krakow.pl](mailto:icavs2023@targi.krakow.pl)

# Honorary Patronage



**Witold Kozłowski**  
The Marshal  
of the Małopolska Region

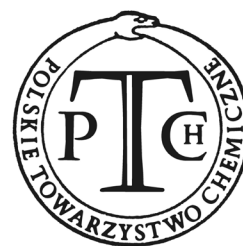


**Jacek Majchrowski**  
The Mayor  
of the City of Krakow



**JAGIELLONIAN UNIVERSITY  
IN KRAKÓW**

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



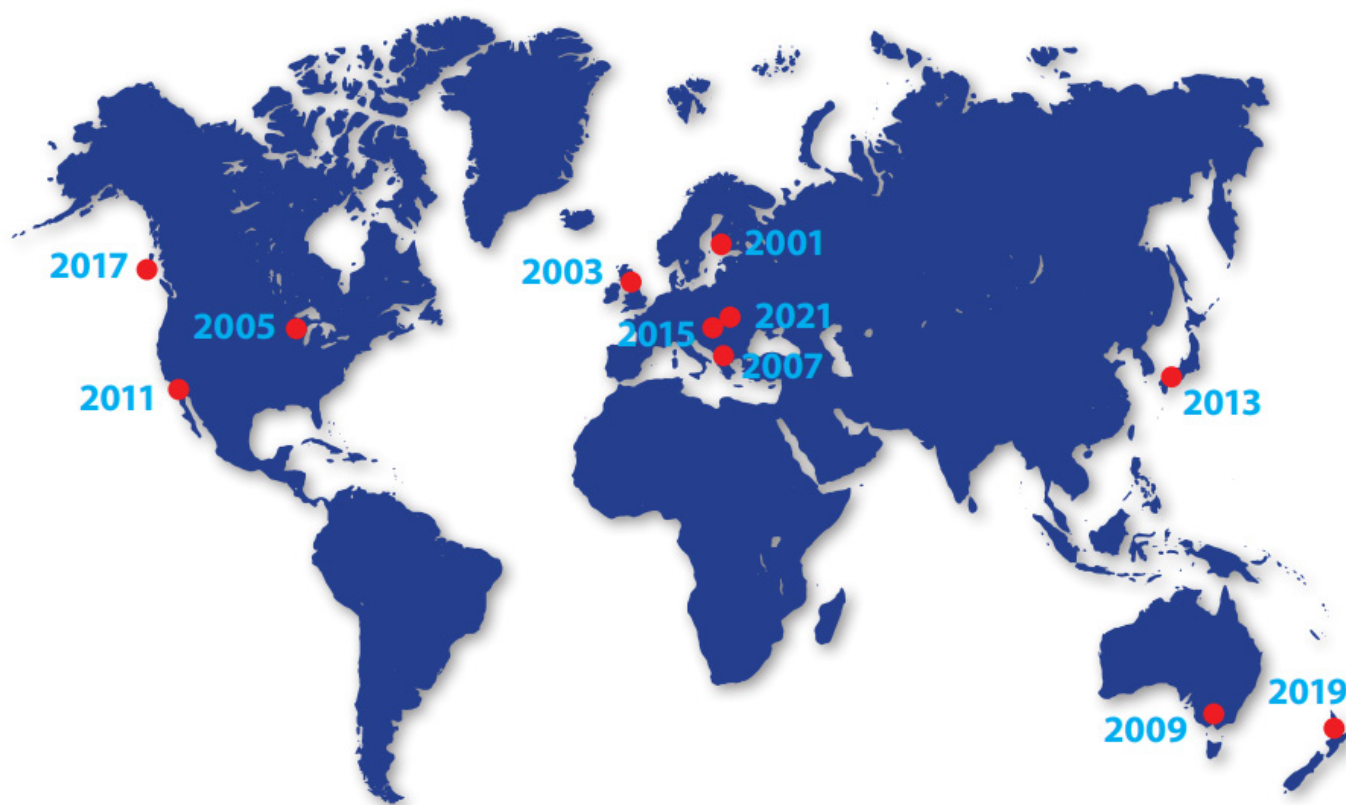
**The Polish  
Chemical Society**



# 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.

CONFERENCE	YEAR	LOCATION	CHAIR	PROGRAM CHAIR
ICAVS1	2001	Turku, Finland	Jyrki Kauppinen	Matti Hotokka
ICAVS2	2003	Nottingham, UK	Michael George	John Chalmers
ICAVS3	2005	Wisconsin, USA	Larry Nafie and Rina Dukor	
ICAVS4	2007	Corfu, Greece	Vasilios Gregariou	Bernhard Lendl
ICAVS5	2009	Melbourne, Australia	Donald McNaughton	Bayden Wood
ICAVS6	2011	California, USA	James de Haseth	Curtis Marcott
ICAVS7	2013	Kobe, Japan	Yukihiro Ozaki	Taskeshi Hasegawa
ICAVS8	2015	Vienna, Austria	Bernhard Lendl	Michael George
ICAVS9	2017	Victoria, Canada	Alexandre Brolo	Dennis Hore
ICAVS10	2019	Auckland, New Zealand	Keith Gordon and Frédérique Vanholsbeeck	Ian R. Lewis and Cushla McGoverin
ICAVS11	2021	Krakow, Poland	Malgorzata Baranska, Kamilla Malek and Katarzyna M. Marzec	Sergei Kazarian
ICAVS12	2023	Krakow, Poland	Kamilla Malek, Malgorzata Baranska and Katarzyna Majzner	Janina Kneipp

# ICAVS12



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 afresh a 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:** zloty (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 zloty (PLN/zł) divided into 100 groszy. Coins come in 1, 2, 5, 10, 20, and 50 groszy, as well as 1, 2, and 5 zloty, while banknotes' denominations note as 10, 20, 50, 100, 200 and 500 zloty. 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 unrepeatable 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/](http://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

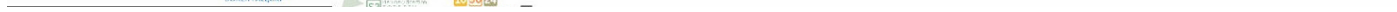
You can take advantage of many local transportation systems in Krakow, such as buses and a wide net of trams. In the very city center, there are plenty of tram and bus lines in service in Krakow that help you get around the city and go beyond its limits (e.g. to Wieliczka). Public transport is organized 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](http://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)



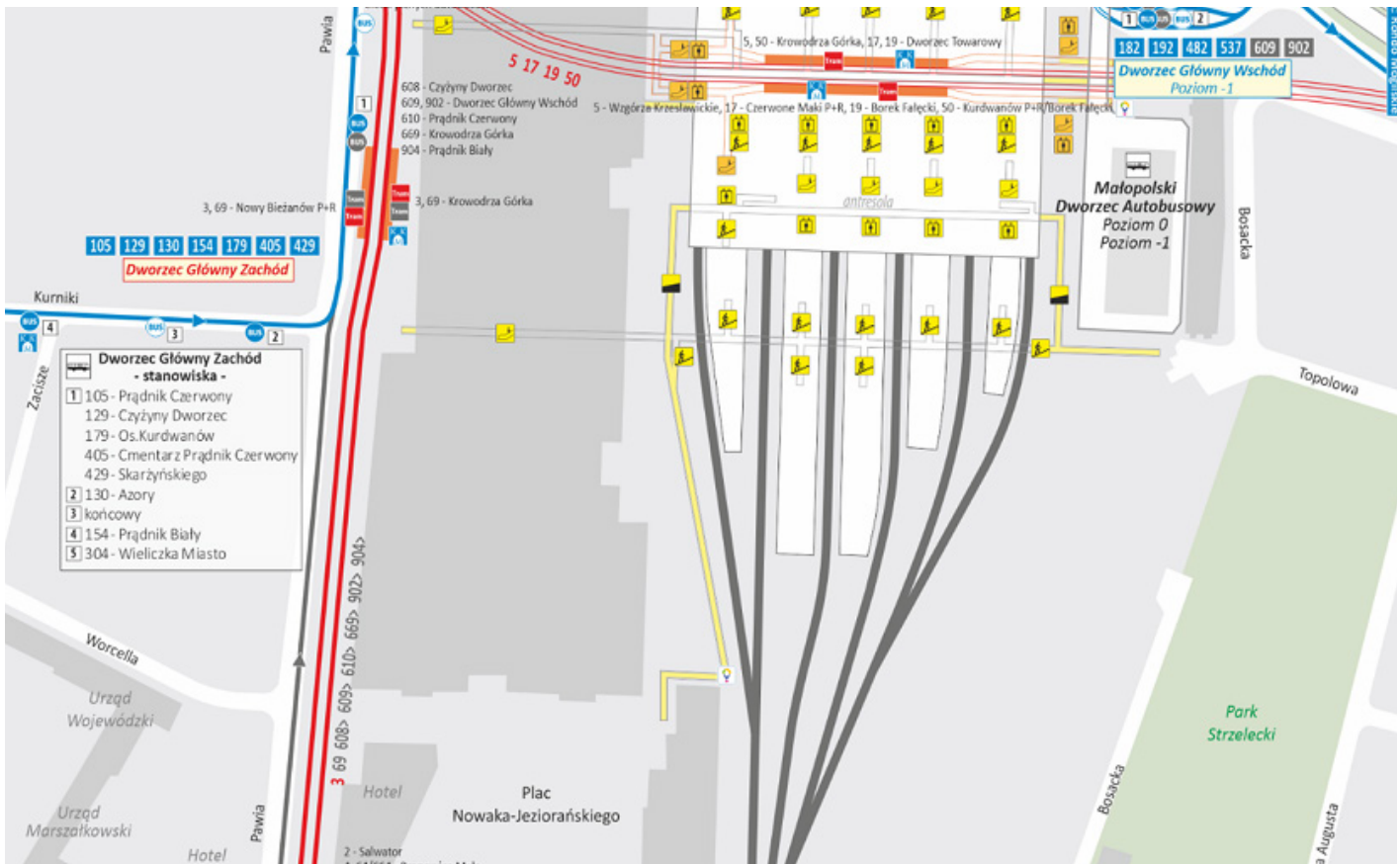
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## Main Railway Station (Dworzec Główny)



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](http://krakowairport.pl), and [kolejemalopolskie.com.pl](http://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](http://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

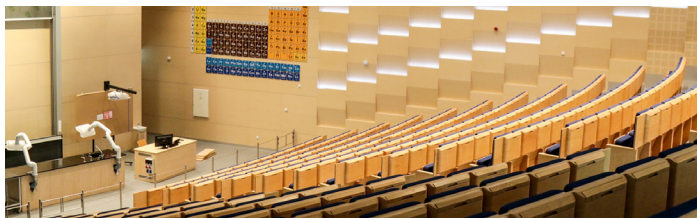
ICAVS 12 will take place in the **Faculty of Chemistry Jagiellonian University (JU) in Krakow (Poland)**, located at the Campus of the **600th Anniversary of the JU Revival on Gronostajowa St. 2, Krakow, Poland**.



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.

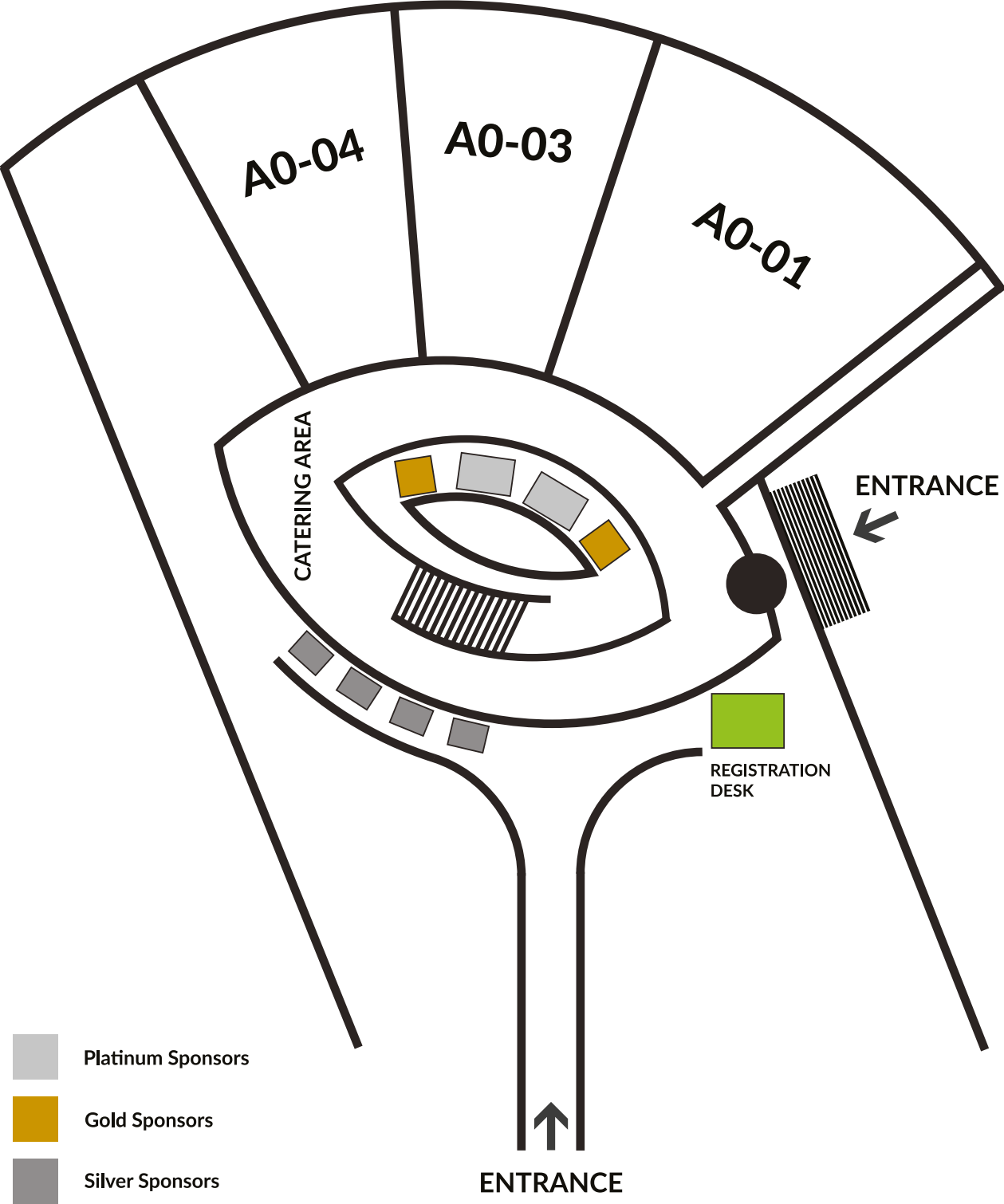
Invited and regular talks will take place in parallel sessions in the lecture halls **A0-01, A0-03, A0-04, A1-01 and A1-02**. Access to lecture halls A1-01 and A1-02 is from the first floor only.

Welcome Cocktail, poster sessions, coffee breaks, and lunches will be held in the exhibition area on the ground and first floor.

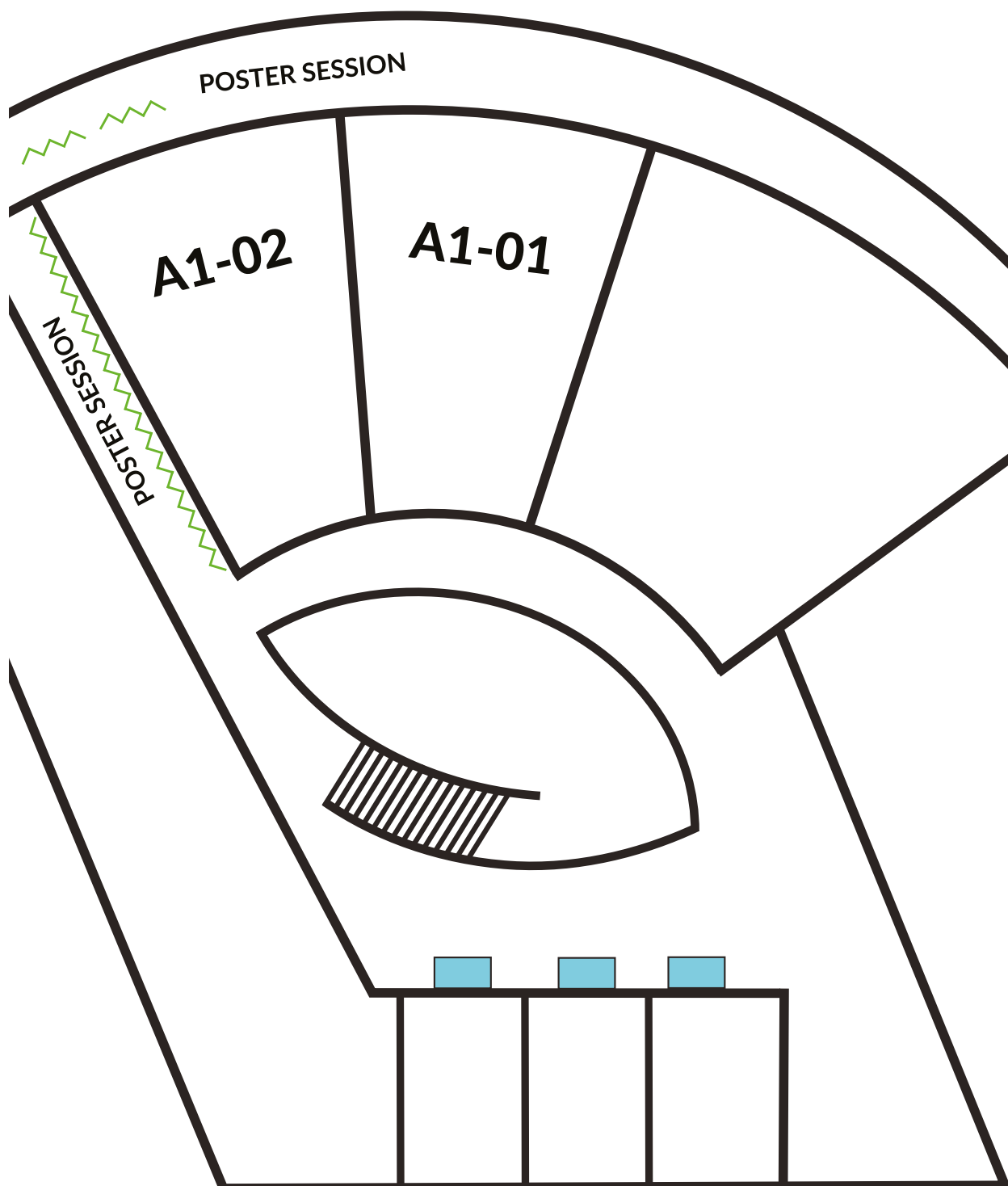




# GROUND FLOOR



# FIRST FLOOR



 Standard Exhibition Space

# 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](http://rozklady.mpk.krakow.pl)

[jakdojade.pl/krakow](http://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**  
MANUFACTURING EXPERTS

## 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 characteristic 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 at 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, participants 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**

## II 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.



## Perspective speakers



**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 Phtalocyanines.

# 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](http://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 CO<sub>2</sub> 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 nano-materials ([www.imperial.ac.uk/vsci](http://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  $\pi$ -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 articles 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

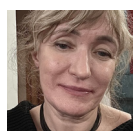
## (A) advanced characterization of organic, inorganic, hybrid, and low-dimensional materials



**Marco Daturi**  
Universite de Caen Normandie  
France



**Christiane Höppener**  
University of Jena  
Germany

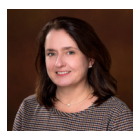


**Joanna Profic-Paczowska**  
Jagiellonian University  
Poland



**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



**Alex Brolo**  
University of Victoria  
Canada



**Laura Fabris**  
Politecnico di Torino  
Italy



**Valeria Giliberti**  
Istituto Italiano di Tecnologia  
Italy



**Malcolm Kadodwala**  
University of Glasgow  
UK



**Maria Rosa Lopez Ramirez**  
University of Malaga  
Spain



**Zachary Schultz**  
Ohio State University  
USA

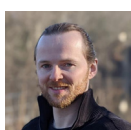


**Hua Zhang**  
Xiamen University  
China

## (D) vibrational spectroscopy of surfaces and interfaces



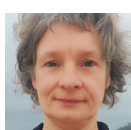
**Patrycja Kielb**  
University of Bonn  
Germany



**Jacek Kozuch**  
Freie Universitat 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

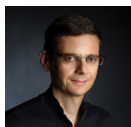


**Kailash Chandra Jena**  
Indian Institute of Technology Ropar  
India



**Dennis Hore**  
University of Victoria  
Canada

## (F) advances in instrumentation



**Krzysztof Banaś**  
National University of Singapore  
Singapore



**Ariane Deniset-Besseau**  
Université Paris-Saclay  
France



**Kishan Dholakia**  
University of St Andrews  
UK



**Torsten Frosch**  
Technische Universität Darmstadt  
Germany

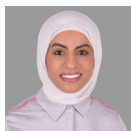


**Bernhard Lendl**  
Technische Universität Wien  
Austria



**Kerstin Ramser**  
Lulea University of Technology  
Sweden

## (G) analytical applications to forensics, PAT, works of art, and similar



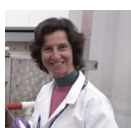
**Entesar Al-Hetlani**  
Kuwait University  
Kuwait



**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

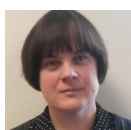
## (H) biomedical/biodiagnostic spectroscopy



**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

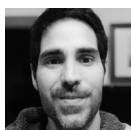


**Fay Nicolson**  
Dana Farber Cancer Institute  
USA



**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

<b>Yiqing Feng</b>	Investigating NBD-Cl and its derivative NBD-Ceramide in living cells using surface enhanced Raman scattering
<b>Tetiana Stepanenko</b>	Molecular Profiling of Erythrocyte Membrane at the Nano-Scale and at the Single Molecule Level
<b>Hadass Tischler</b>	Super-Resolution Raman Spectroscopy—Applications to Diamond Identification
<b>Martina Zangari</b>	FTIR microscopy and nanoscopy analysis of protein- fiber interaction in asbestos body model assembling

## Session B

<b>Maxim Bokov</b>	Rearrangement of intracellular crystalline guanine as an adaptation for various illumination levels
<b>Agnieszka Domagała</b>	Protein structure investigation via ROA-CPL spectroscopy and Eu(III) probe
<b>Andrea Dali</b>	Spectroscopic characterization of the coproporphyrin ferrochelatase from <i>Corynebacterium diphtheriae</i>
<b>Monika Hałat</b>	Raman Optical Activity is a sensitive tool to detect changes in the structure of biomolecules and supramolecules
<b>Štěpán Jílek</b>	Formation and Behavior of Guanosine-5'-Monophosphate assemblies at low pH: temperature and cation effects
<b>Chara Karafoulidi-Retsou</b>	Characterizing the large subunit of a membrane-bound [NiFe] hydrogenase by combined IR spectroscopic and computational studies
<b>Petra Maleš</b>	The revelation of interactions in model myelin with FTIR spectroscopy
<b>Fatima Matroodi</b>	Spectral features of Interfacial Water in Imidazolium-based Ionic Liquids/water mixtures: UV Resonance Raman Approach
<b>Katarzyna Pajor</b>	How to properly register Raman optical activity spectra of chiral and light-absorbing biomolecules?
<b>Sung Man Park</b>	Conformational study by IR resonant VUV-MATI mass spectroscopy
<b>Patryk Pyrcz</b>	Temporal Evolution of Single-Molecule Surface-Enhanced Raman Scattering Spectra
<b>Naoki Sakurai</b>	Conformation of choline-chloride-based deep eutectic solvents and its temperature dependence observed with Raman spectroscopy
<b>Věra Schrenková</b>	Characterization of sofosbuvir polymorphs using polarized Raman microscopy
<b>Cecilia Spedaliere</b>	UV resonance Raman of serum albumins
<b>Risa Suzuki</b>	Formation of vitamin D3 observed by picosecond time-resolved Raman spectroscopy

## Session C

<b>Cherine Alaouta</b>	Development of high-Throughput Raman imaging to investigate the efficacy of Doxifluridine Squalenoyl nanomedicine on single breast cancer cells
<b>Shrobona Banerjee</b>	Surface-enhanced Raman scattering (SERS) of biomolecules - Can the variations tell a story?

<b>Ioana Marica</b>	Optical properties and SERS analysis of quasi-3D plasmonic nanostructures fabricated by colloidal lithography
<b>Beata Wrzosek</b>	A new approach in the SERS blinking analysis
<b>Session D</b>	
<b>Ilijana Bajama</b>	Dual-tag paradigm in SERS analysis for removal of antibiotics and dyes from waste water treated with biogenic carbonate powder nanoparticles
<b>Yi-Fan Bao</b>	AFM-based non-gap mode tip-enhanced Raman spectroscopy (TERS)
<b>Amanda Bartkowiak</b>	Application of Resonance Raman Spectroscopy for label-free differentiation of ferrous and ferric cytochrome c
<b>Lars Dannenberg</b>	Monitoring plasmon-mediated chemical reactions on immobilized noble metal nanoparticles
<b>Paul Kerner</b>	Atomic-scale dynamics in plasmonic hotspots: fast SERS of picocavities
<b>Adrian Warzybok</b>	Photo-induced enhanced Raman spectroscopy on thin Ag-TiO <sub>2</sub> nanoplateforms: a study of mechanisms and influence of visible light
<b>Li Zhang</b>	Understanding Structure, Interference, and Absorption effects in Vibrational SFS Experiments
<b>Session E</b>	
<b>Aruna Kumarasiri</b>	Electronic Structure of para-Cyanophenol at the Air-Aqueous Interface from Vibrational Sum Frequency Generation Spectroscopy
<b>Session F</b>	
<b>Shiwani</b>	High-Throughput Raman System for Rapid Microplastic Characterization
<b>Session G</b>	
<b>Meshari Al-Qalfas</b>	Assessment of the effects of Kuwait's high temperatures and humidity on whole blood stains stability on fabric using ATR-FTIR spectroscopy
<b>Loren Christie</b>	Cell metabolite quantification using the Dxcover infrared platform
<b>Víctor Navarro Esteve</b>	Poc quantification and profiling of urine cells by integrating cytocentrifugation and ir measurements on the same substrate
<b>Felix Frank</b>	A new sensitive multi-analyte VOC sensor based on an integrated optics waveguide coated with a functionalised mesoporous sensing layer and QCL-IR spectrometry
<b>Jiro Karlo</b>	Exploring potential of reverse Raman Stable Isotope Probing and 2D correlation spectroscopy in monitoring metabolic pathway dynamics in situ.
<b>Alžbeta Kuižová</b>	Drop coating deposition Raman spectroscopy (DCDRS) as a tool for rapid determination and identification of contaminants and food additives
<b>Marika Niihori</b>	Towards the intelligent toilet: SERS sensing of nM-level neurotransmitters with Fe-sensitized self-assembled gold nanoparticle arrays
<b>Shravan Raghunathan</b>	Bio-chemical assessment of blood cell and PBMC smears using optical photothermal mid-IR spectroscopy for studies of diseases and infections
<b>Gohar Soufi</b>	Identification and classification of methotrexate and its metabolites in human serum samples using surface-enhanced Raman scattering combined with advanced data analysis



<b>Chiaramaria Stani</b>	FTIR nano-spectroscopy at SISSI-Bio Beamline: recent insight in the field of Cultural Heritage
<b>Session H</b>	
<b>Masoumeh Alinaghi</b>	Strong impact of de novo purine biosynthesis on the spectroscopic signature of <i>Staphylococcus aureus</i> revealed by the screening of a gene-defined transposon mutant library
<b>Helena Friedrich</b>	Metabolic impacts of microplastic exposure in mammalian cells measured via FTIR microspectroscopy
<b>Wiktorja Korona</b>	Non-label identification of acute myeloid leukemia with FLT3 gene mutation using Raman spectroscopy
<b>Mateusz Migdalski</b>	Raman and Resonance Raman Spectroscopy for Malaria Red Blood Cells Analysis
<b>Muhammad</b>	SERS-imaging for probing program death ligand-1 immunomarker in real-time tumour progression
<b>Aleksandra Pragnaça</b>	Spectroscopic detection of hypoxic state in the brain endothelium and endothelial progenitor cells
<b>Ota Samek</b>	Effects of antimicrobials on microbial Raman spectra as the first step for detection of antimicrobial resistance
<b>Kacper Siąkała</b>	Spectroscopic analysis of the fatty acids uptake by human leukemic cells and accompanying metabolic changes
<b>Kacper Stawowski</b>	Differentiation and classification of leukemic cells with the use of Raman Imaging
<b>Jizhou Zhong</b>	Discovery of novel spectral biomarkers for early diagnosis of Lyme Disease
<b>Session I</b>	
<b>Tarek Eissa</b>	In silico modeling reveals the prospects and limitations of vibrational fingerprinting for phenotyping biological systems
<b>Jaume Béjar Grimalt</b>	Monitoring of physical effort by infrared spectroscopy of urine composition
<b>Azadeh Mokari</b>	Pre-processing Raman data via deep learning method
<b>Session J</b>	
<b>Julian Mateo Rayo Alape</b>	Vibrational calculations and SERS activity prevision of hepcidin hormone: contribution for hyperinflammation screening
<b>Corentin Grassin</b>	IR/VCD spectroscopic studies on matrix-isolated chiral 1-phenyl-1-propanol
<b>Jana Hudecová</b>	Structure of Histidine-Metal Complexes in Solution Revealed by Raman Optical Activity
<b>Mohammed Siddhique Para Kkadan</b>	Development of Computational Models to Decipher Raman Optical Activity Spectra of G-quadruplexes

# Program

Sunday	11:00-20:00	Registration			
	11:30-17:10	Workshop Session			
	WORKSHOP SESSION	11:30-13:30 Workshop session 1 (Horiba) ROOM: A0-01 13:30-15:30 Workshop session 2 (WiTec - ROOM: A0-03, Photothermal - ROOM: A0-04) 15:30-17:15 CLIRSPEC session ROOM: A0-01   Chairs: Peter Gardner, Hugh Byrne			
	17:00-17:30	Coffee break			
	17:30-19:30	Perspective Session ROOM: A0-01   Chairs: Kamilla Malek, Malgorzata Baranska, Janina Kneipp, Katarzyna Majzner			
Monday	PERSPECTIVE SESSION	17:30-17:55 K.M. Gough <i>Progress in infrared spectroscopy</i> 18:05-18:30 L.A. Nafe <i>Frontiers of Advanced Vibrational Spectroscopy: The Molecular Chirality Perspective</i> 18:40-19:05 G. Smulevich <i>Strategies and perspectives to investigate the heme-enzymatic mechanism by resonance Raman spectroscopy</i>			
	19:30-21:30	Welcome Cocktail – Conference Venue			
	8:45-9:00	Opening Ceremony			
	9:00-10:15	Plenary Session ROOM: A0-01			
	PLENARY SESSION	9:00-9:30 A. Rodger <i>Can attenuated total reflectance infrared spectroscopy (ATR-IR) be used with polarized light?</i>   Chair: Bin Ren 9:40-10:10 A. R. Hight Walker <i>In-Operando Magneto-Raman Study of Graphene Device in the Quantum Hall Regime</i>   Chair: Harumi Sato			
Tuesday	10:15-10:45	Coffee Break			
	10:45-12:10	SESSION 1			
	SESSION 1	Chair: Ewan Blanch (B) <i>Structure&amp;dynamics of molecules</i> ROOM: A1-01	Chair: Volker Deckert (C) <i>Spectroscopy in local fields</i> ROOM: A1-02	Chair: Kerstin Ramser (F) <i>Advances in instrumentation</i> ROOM: A0-04	Chair: Young-Mee Jung (G) <i>Analytical applications</i> ROOM: A0-03
		10:45-11:00 P. Mak	10:45-11:00 V. Giliotti	10:45-11:00 K. Banas	10:45-11:00 A. Kaminska
		11:05-11:20 B. Rossi	11:05-11:20 M. Kadodwala	11:05-11:20 A. Deniset-Besseau	11:05-11:20 L. Vaccari
		11:25-11:35 J. Drybaś	11:25-11:35 H. Bechtel	11:25-11:35 O. Alshareef	11:25-11:35 D. Cialla-May
		11:40-11:50 K. Dziedzic-Kocurek	11:40-11:50 N. Stone	11:40-11:50 N. Lenngren	11:40-11:50 J. Udensi
		11:55-12:05 M. Horch		11:55-12:05 M. Roman	11:55-12:05 E. Wyatt
	12:10-13:10	Lunch			
	13:10-14:35	SESSION 2			
	SESSION 2	Chair: Federica Piccirilli (B) <i>Structure&amp;dynamics of molecules</i> ROOM: A1-01	Agata Królkowska (C) <i>Spectroscopy in local fields</i> ROOM: A1-02	Chair: Agnieszka Banas (F) <i>Advances in instrumentation</i> ROOM: A0-04	Chair: Yaakov Tischler (G) <i>Analytical applications</i> ROOM: A0-03
		13:10-13:25 L. Webb	13:10-13:25 A. Brolo	13:10-13:20 H. Butler	13:10-13:20 K. Augustyniak
		13:30-13:45 T. Weidner / F. Madzharova	13:30-13:45 Z. Schultz	13:25-13:35 A. Cernescu	13:25-13:35 A.L.M. Batista de Carvalho
		13:50-14:00 K. Cieřlik-Boczula	13:50-14:00 C. Deriu	13:40-13:50 M. Godejohann	13:40-13:50 H.M. Heise
		14:05-14:15 P. Mojeř	14:05-14:15 S. Gawinkowski	13:55-14:05 M. Unger	13:55-14:05 V. Notarstefano
			14:20-14:30 W.K. Son		14:10-14:20 A. Sroka-Bartnicka
					14:25-14:35 Y. Wang
	14:30-15:00	Coffee Break			
	15:00-16:15	SESSION 3			
	SESSION 3	Chair: Piotr Mak (B) <i>Structure&amp;dynamics of molecules</i> ROOM: A1-01	Chair: Zachary Schultz (C) <i>Spectroscopy in local fields</i> ROOM: A1-02	Chair: Holly Butler (F) <i>Advances in instrumentation</i> ROOM: A0-04	Chair: Cassio Lima (G) <i>Analytical applications</i> ROOM: A0-03
		15:00-15:10 L. Goett-Zink	15:00-15:15 H. Zhang	15:00-15:15 K. Dholakia	15:00-15:10 A. Arbiol
		15:15-15:25 T. Kottke	15:20-15:35 J. Baumberg	15:20-15:35 T. Frosch	15:15-15:25 C. Kamp
		15:30-15:40 H. Ma / X.Wang	15:40-15:50 O. Garrity	15:40-15:50 V. Deckert	15:30-15:40 C. Liu
		15:45-15:55 K.M. Marzec	15:55-16:05 A. Mahmoud	15:55-16:05 M. Ortolani	15:45-15:55 G. Tyagi
		16:00-16:10 S. Morita	16:10-16:20 E. Kořisova	16:10-16:20 S. Bernatová	16:05-16:15 H. Jin
	16:30-18:45	POSTER SESSION 1			
	FLASH & POSTER SESSION	16:30-17:30 Flash Presentations (Topics A-F, J) ROOM: A0-01   Chairs: Lisa Vaccari, Shigeaki Morita			
		17:30-18:45 Poster Session (Topics B-D)			
	18:00-18:45	Steering Committee meeting			
Wednesday	9:00-10:15	Plenary Session ROOM: A0-01			
	PLENARY SESSION	9:00-9:30 K. Iwata <i>Bimolecular chemical reactions in solution examined with time-resolved infrared and Raman spectroscopy</i>   Chair: Giulietta Smulevich 9:40-10:10 D. Kim <i>Ultrafast Structural Dynamics in Various <math>\pi</math>-Conjugated Molecular Systems Probed by Time-resolved Electronic and Vibrational Spectroscopy</i>   Chair: Yukihiro Ozaki			
	10:15-10:45	Coffee Break			
	10:45-12:10	SESSION 1			
	SESSION 1	Chair: Valeria Giliotti (B) <i>Structure&amp;dynamics of molecules</i> ROOM: A1-01	Chair: Eva Kořisová (C) <i>Spectroscopy in local fields</i> ROOM: A1-02	Chair: Wojciech Kwiatek (F) <i>Advances in instrumentation</i> ROOM: A0-04	Chair: Entesar Al-Hetlani (G) <i>Analytical applications</i> ROOM: A0-03
		10:45-11:00 P. Hellwig	10:45-11:00 L. Fabris	10:45-10:55 M. Kansiz	10:45-10:55 G. Birarda
		11:05-11:20 J. Wang	11:05-11:20 M.R. López-Ramírez	11:00-11:10 J. Kapitán	11:00-11:10 J. Chwiej
		11:25-11:35 F. Piccirilli	11:25-11:35 A. Królkowska	11:15-11:25 B.J.A. Mooij	11:15-11:25 M. Krysa
		11:40-11:50 K. Sofinska	11:40-11:50 X. Yao	11:30-11:40 J. Diniz	11:30-11:40 J. Landry
			11:55-12:05 Ł. Pięta	11:45-11:55 K. Stergiou	11:45-11:55 Y. Ozaki
				12:00-12:10 A. Whitley	12:00-12:10 M. Pucateita
	12:10-13:10	Lunch			
	13:15-14:30	POSTER SESSION 2			
	FLASH & POSTER SESSION	13:15-14:30 Poster Session (Topics A, E, F, J)			
Thursday	14:45-18:00	Excursion			
	19:00	Beer Club			
Friday	9:00-10:15	Plenary Session			
	PLENARY SESSION	9:00-9:30 S.G. Kazarian <i>Advances in Infrared Spectroscopic Imaging</i>   Chair: Kathleen Gough 9:40-10:10 J. Weinstein <i>Towards vibrational control of electron transfer with short IR pulses</i>   Chair: Christian Huck			
	10:15-10:45	Coffee Break			
	10:45-12:10	SESSION 1			
	SESSION 1	Chair: Judith Mihály (B) <i>Structure&amp;dynamics of molecules</i> ROOM: A1-01	Chair: Freek Ariese (E) <i>Nonlinear vibrational spectroscopy</i> ROOM: A1-02	Chair: Yuzuke Moricawa (F) <i>Advances in instrumentation</i> ROOM: A0-04	Chair: Maria Lopez-Ramirez (G) <i>Analytical applications</i> ROOM: A0-03
		10:45-10:55 E. Blanch	10:45-11:00 Z. Heiner	10:45-11:00 B. Lendl	10:45-11:00 K. Gordon
		11:00-11:10 M. Czarniecki	11:05-11:20 K. Hiramatsu	11:05-11:20 K. Ramser	11:05-11:20 M.P. Marques
		11:15-11:25 E. Machalska	11:25-11:35 A. Geddis	11:25-11:35 K. Brzozowski	11:25-11:35 A. Antolak
		11:30-11:40 C. Malherbe	11:40-11:50 F. Madzharova	11:40-11:50 M. Huber	11:40-11:50 A. Banas
		11:45-11:55 V. Profant	11:55-12:05 M. Zelenka	11:55-12:05 Ch. W. Huck	11:55-12:05 D. Święch
	12:10-13:10	Lunch			
	13:10-14:30	SESSION 2			
	SESSION 2	Chair: Katarzyna Cieřlik-Boczula (I) <i>Chemometrics&amp;machine learning</i> ROOM: A1-01	Chair: Xiang Wang (E) <i>Nonlinear vibrational spectroscopy</i> ROOM: A1-02	Chair: Yuling Wang (F) <i>Advances in instrumentation</i> ROOM: A0-04	Chair: Natalia Ivleva (G) <i>Analytical applications</i> ROOM: A0-03
		13:10-13:25 B. Kupcewicz	13:10-13:25 J. Gibbs	13:10-13:20 A. Dabrowska	13:10-13:20 K.B. Bec
		13:30-13:40 U. Blazhko/ Magnussen	13:30-13:45	13:25-13:35 H. Hiramatsu	13:25-13:35 K. Beton-Mysur
		13:45-13:55 M. De Gá Neves	13:50-14:00 F. Bell	13:40-13:50 O. Ilchenko	13:40-13:50 M. Konings
		14:00-14:10 M. A. M. Nowakowska	14:05-14:15 M. Pastorcak	13:55-14:05 C. Neuper	13:55-14:05 C. Lima
			14:20-14:30 L. Zada	14:10-14:20 A. Sacco	14:10-14:20 G. Ramer
				14:25-14:35 I. Zeliger	14:25-14:35 I. Yoshikawa
	14:30-15:00	Coffee Break			
	15:00-16:15	SESSION 3			
	SESSION 3	Chair: Stefania Dana Iancu (I) <i>Chemometrics&amp;machine learning</i> ROOM: A1-01	Chair: Marcin Pastorcak (E) <i>Nonlinear vibrational spectroscopy</i> ROOM: A1-02	Chair: Justyna Grabska (A) <i>Advanced characterization of materials</i> ROOM: A0-04	Chair: Maria-Paula Marques (G) <i>Analytical applications</i> ROOM: A0-03
		15:00-15:10 J.E. Clément	15:00-15:10 F. Ariese	15:00-15:15 C. Höppener	15:00-15:15 E. Al-Hetlani
		15:15-15:25 E. Harju	15:15-15:25 A. Borek-Dorosz	15:20-15:35 M. Procházka	15:20-15:35 B. Wood
		15:30-15:40 P. Leszczenko	15:30-15:40 R. Eriksson	15:40-15:50 S. Katz	15:40-15:50 M.O. Amin
		15:45-15:55 S. Mostafapour	15:45-15:55 A. Pieczara	15:55-16:05 Y.R.Tischler	15:55-16:05 A. Wójtowicz
		16:00-16:10 M. Zigman	16:00-16:10 J. Saarinen		15:45-15:55 S. Orzechowska
					16:00-16:10 L. Pioppi
	16:30-18:45	POSTER SESSION 3: Topics G, H, I			
	FLASH & POSTER SESSION	16:30-17:30 Flash Presentations ROOM: A0-01   Chairs: Sara Miller, Christian Johannessen			
		17:30-18:45 Poster Session			

Thursday	9:00-10:15	Plenary Session ROOM: A0-01				
	PLENARY SESSION	9:00-9:30 N. Gierlinger <i>Raman Imaging of Plant Cells: probing distribution and orientation of molecules</i>   Chair: Pavel Matousek 9:40-10:10 A. Mosig <i>Theory is dead, long live theory: Hypothesis-centric machine learning in vibrational spectroscopy</i>   Chair: Petra Hellwig				
	10:15-10:45	Coffee Break				
	10:45-12:10	SESSION 1				
		Chair: Alicja Dąbrowska (I) <i>Chemometrics&amp;machine learning</i> ROOM: A1-01	Chair: Zsuzsanna Heiner (E) <i>Nonlinear vibrational spectroscopy</i> ROOM: A1-02	Chair: Valentina Notarstefano (A) <i>Advanced characterization of materials</i> ROOM: A0-04	Chair: Inez Weidinger (D) <i>Spectroscopy of surface&amp;interfaces</i> ROOM: A0-03	Chair: Michael Heise (H) <i>Biological spectroscopy</i> ROOM: A0-01
		10:45-10:55 M. Chalmers	10:45-11:00 D. Hore	10:45-10:55 B. Gieroba	10:45-11:00 P. Kielb	10:45-11:00 B. Brozek-Pluska
		11:00-11:10 A. Kalka	11:05-11:20 S. Nihonyanagi	11:00-11:10 S. Miller	11:05-11:20 B. Ren	11:05-11:20 Hidetoshi Sato
		11:15-11:25 A. Masella	11:25-11:35 S. Kaur	11:15-11:25 G.P. Szekeres	11:25-11:35 M. Borrelli	11:25-11:35 K. Karpienko
		11:30-11:40 A. Kutyk	11:40-11:50 E. Mai	11:30-11:40 E. Tay	11:40-11:50 X. Wang	11:40-11:50 C. Morasso
		11:45-11:55 M. Poth	11:55-12:05 S. Pullanchery	11:45-11:55 A. Kolodziej	11:55-12:05 F. Aguiar Junior	11:55-12:05 M. Ventura
		12:00-12:10 R. Schmidt		12:00- 12:10 A. Weselucha-Birczyńska		
	12:10-13:10	Lunch				
	13:10-14:30	SESSION 2				
		Chair: Valeria Tafintseva (I) <i>Chemometrics&amp;machine learning</i> ROOM: A1-01	Chair: James Cheeseman (J) <i>Computational approaches</i> ROOM: A1-02	Chair: Ana Batista de Carvalho (A) <i>Advanced characterization of materials</i> ROOM: A0-04	Chair: Ahmad Salman (D) <i>Spectroscopy of surface&amp;interfaces</i> ROOM: A0-03	Chair: Josep Sule-Suso (H) <i>Biological spectroscopy</i> ROOM: A0-01
Friday		13:10-13:20 R. Cheng	13:10-13:25 P. Bour	13:10-13:20 M. Bik	13:10-13:25 J. Kozuch	13:10-13:20 D.E. Bedolla
		13:25-13:35 G.R. Dewantier	13:30-13:45 J.E. Rode	13:25-13:35 N. Ivleva	13:30-13:45 H.K. Ly	13:25-13:35 K. Chrabaszcz
		13:40-13:50 S. Diehn	13:50-14:00 Y. Morisawa	13:40-13:50 M. Saad	13:50-14:00 E. Lipiec	13:40-13:50 C. Combescot
		13:55-14:05 D. Kavungal	14:05-14:15 S. Jähnigen	13:55-14:05 Harumi Sato	14:05-14:15 N. Piergies	13:55-14:05 L. Lovergne
		14:10-14:20 A. Laubscher	14:20-14:30 S. Kanugula	14:10-14:20 T. Wrobel		14:10-14:20 E. Pięta
		14:25-14:35 C. Pereira	14:35-14:45 T. Mayerhöfer			14:25-14:35 P. Sassi
	14:45-15:00	SHIM-POL presentation ROOM A0-01				
	18:30 (assembly 17:30)	Conference Dinner				
	9:00-10:15	Plenary Session ROOM: A0-01				
	PLENARY SESSION	9:00-9:30 J. Aizpurua <i>Molecular Optomechanics Approach to Surface-Enhanced Raman Scattering</i>   Chair: Alexandre Brolo 9:40-10:10 R. Bhargava <i>Increasing utility of IR imaging by high performance instrumentation and AI</i>   Chair: Katarzyna Marzec				
	10:15-10:45	Coffee Break				
	10:45-12:10	SESSION 1				
		Chair: Milda Pucetaite (I) <i>Chemometrics&amp;machine learning</i> ROOM: A1-01	Chair: Thomas Mayerhöfer (J) <i>Computational approaches</i> ROOM: A1-02	Chair: Sagie Katz (A) <i>Advanced characterization of materials</i> ROOM: A0-04	Chair: Cecilia Spedalieri (D) <i>Spectroscopy of surface&amp;interfaces</i> ROOM: A0-03	Chair: Bayden Wood (H) <i>Biological spectroscopy</i> ROOM: A0-01
		10:45-11:00 D. Pérez-Guaita	10:45-10:55 J. Cheeseman	10:45-11:00 M. Daturi	10:45-11:00 J. Langer	10:45-11:00 B. Gardner
		11:05-11:20 V. Tafintseva	11:00-11:10 C. Johannessen	11:05-11:20 J. Profic-Paczkowska	11:05-11:15 J. Mihály	11:05-11:15 N. Leopold
		11:25-11:35 ES. Lehner	11:15-11:25 V. Liegeois	11:25-11:35 B. Bracco	11:20-11:30 K. Pogoda	11:20-11:30 S. Mazurek
		11:40-11:50 D. Liberda	11:30-11:40 J. Grabska	11:40-11:50 M. Gawęda	11:35-11:45 S.D. Iancu	11:35-11:45 A. Salman
		11:55-12:05 E.A. Magnussen	11:45-11:55 G. Zając			
	12:10-12:45	Award&Closing Ceremony ROOM: A0-01				
		12:10-12:20 ICAVS Awards				
		12:20-12:30 Introduction of ICAVS 13				
		12:30-12:45 Summary of ICAVS 12 and Good Bye				
	12:45-13:45	Lunch				

# Detailed program

Sunday		
11:00-20:00		Registration
11:30-17:15	Room	Workshop Session
11:30-13:30	A0-01	Workshop session 1 HORIBA/COMEF <b>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.</b>
13:30-15:30	A0-03	Workshop session 2 WITec Raman Workshop <b>New Perspectives in 3D Raman Imaging and Correlative Techniques</b>
13:30-15:30	A0-04	Workshop session 2 Photothermal: O-PTIR Workshop <b>Submicron IR and Simultaneous Raman Microscopy with Co-Located Fluorescence Imaging</b>
15:30-17:15	A0-01	CLIRSPEC session   Chairs: Peter Gardner, Hugh Byrne
17:00-17:30		Coffee break
17:30-19:30	A0-01	Perspective Session Chairs: Kamilla Malek, Małgorzata Baranska, Janina Kneipp, Katarzyna Majzner
17:30-17:55	A0-01	Progress in infrared spectroscopy Kathleen Gough <sup>1</sup> <sup>1</sup> University of Manitoba
18:05-18:30	A0-01	Frontiers of Advanced Vibrational Spectroscopy: The Molecular Chirality Perspective Laurence Nafie <sup>1</sup> <sup>1</sup> Syracuse University
18:40-19:05	A0-01	Strategies and perspectives to investigate the heme-enzymatic mechanism by resonance Raman spectroscopy Giulietta Smulevich <sup>1</sup> <sup>1</sup> Dipartimento di Chimica "Ugo Schiff" (DICUS), Università di Firenze
19:30-21:30		Welcome Cocktail – Conference Venue
8:45-9:00	A0-01	Opening Ceremony
Monday		
9:00-10:15	A0-01	Plenary Session Chairs: Bin Ren, Harumi Sato
9:00-9:30	A0-01	Can attenuated total reflectance infra red spectroscopy (ATR-IR) be used with polarised light? Alison Rodger <sup>1</sup> , Paul Wormell <sup>2</sup> , Jun Koshub <sup>3</sup> , Junya Kitamura <sup>3</sup> , Akihiro Sato <sup>3</sup> <sup>1</sup> Macquarie University <sup>2</sup> Western Sydney University <sup>3</sup> Jasco International
9:40-10:10	A0-01	In-Operando Magneto-Raman Study of Graphene in the Quantum Hall Regime Angela Hight Walker <sup>1</sup> <sup>1</sup> National Institute of Standards and Technology (NIST)
10:15-10:45		Coffee Break
10:45-12:10		SESSION 1
	A1-01	(B) Structure&dynamics of molecules Chair: Ewan Blanch
10:45-11:00		Probing the active site structural changes in P450/P420 forms of CYP121 Piotr Mak <sup>1</sup> <sup>1</sup> Saint Louis University
11:05-11:20		Insights into molecules structure and dynamics by multi-wavelengths UV Resonance Raman spectroscopy Barbara Rossi <sup>1</sup> <sup>1</sup> Elettra Sincrotrone Trieste

11:25-11:35		<b>Detection, characterization, and differentiation of SHb and HbFeIII-SH adducts inside functional erythrocytes</b> <u>Jakub Dybaś<sup>1</sup>, Tetiana Stepanenko<sup>2</sup>, Grzegorz Zajac<sup>1</sup>, Katarzyna M. Marzec<sup>3</sup></u> <sup>1</sup> Jagiellonian University, Jagiellonian Centre for Experimental Therapeutics (JCET) <sup>2</sup> Solaris National Synchrotron Radiation Centre, Jagiellonian University <sup>3</sup> AGH University of Science and Technology 3. Mot, A. C., Puscas, C., Dorneanu, S. A., & Silaghi-Dumitrescu, R. (2019). EPR detection of sulfanyl radical during sulfhemoglobin formation – Influence of catalase. Free Radical Biology and Medicine, 137, 110–115.DOI: 10.1016/j.freeradbiomed.2019.04.034
11:40-11:50		<b>Revealing the problem of the effective charge of iron ion in oxy-haemoglobin molecule</b> <u>Katarzyna Dziedzic-Kocurek<sup>1</sup>, Jakub Dybaś<sup>2</sup>, Jan Stanek<sup>1</sup></u> <sup>1</sup> Faculty of Physics, Astronomy and Applied Computer Science, M. Smoluchowski Institute of Physics, Jagiellonian University
11:55-12:05		<b>Understanding Hydrogenases by 2D-IR Spectroscopy and Vibrational Perturbation Theory</b> <u>Marius Horch<sup>1</sup>, Yvonne Rippers<sup>1</sup>, Cornelius Bernitzky<sup>1</sup>, Solomon Wrathall<sup>2</sup>, Barbara Procacci<sup>2</sup>, Janna Schoknecht<sup>3</sup>, Claudia Schulz<sup>3</sup>, Christian Lorent<sup>3</sup>, Catharina Kulka-Peschke<sup>3</sup>, James Birrell<sup>4</sup>, Ingo Zebger<sup>3</sup>, Gregory Greetham<sup>5</sup>, Oliver Lenz<sup>3</sup>, Neil Hunt<sup>2</sup></u> <sup>1</sup> Freie Universitaet Berlin <sup>2</sup> University of York <sup>3</sup> Technische Universitaet Berlin <sup>4</sup> University of Essex <sup>5</sup> Rutherford Appleton Laboratory
	A1-02	<b>(C) Spectroscopy in local fields</b> Chair: Volker Deckert
10:45-11:00		<b>Probing protein conformations at the nanoscale by means of IR nanospectroscopy</b> <u>Antonia Intze<sup>1</sup>, Maria Eleonora Temperini<sup>1</sup>, Raffaella Polito<sup>2</sup>, Michele Ortolani<sup>2</sup>, Valeria Giliberti<sup>3</sup></u> <sup>1</sup> Istituto Italiano di Tecnologia, Center for Life Nano- and Neuro-Science <sup>2</sup> Department of Physics, Sapienza University of Rome <sup>3</sup> Istituto Italiano di Tecnologia, Center for Life Nano- and Neuro-Science
11:05-11:20		<b>Nanophotonic platforms for enhanced chirally sensitive vibrational spectroscopy</b> <u>Malcolm Kadodwala<sup>1</sup></u> <sup>1</sup> University of Glasgow
11:25-11:35		<b>Viewing interfacial chemistry through a graphene window with broadband infrared nanospectroscopy</b> <u>Hans Bechtel<sup>1</sup>, Jonathan Larson<sup>2</sup>, Xiao Zhao<sup>3</sup>, Xin He<sup>2</sup>, Dong Li<sup>4</sup>, Behzad Rad<sup>4</sup>, Chunsheng Yan<sup>4</sup>, Paul Ashby<sup>4</sup>, Stephanie Gilbert Corder<sup>1</sup>, Robert Kostecki<sup>2</sup>, Miquel Salmeron<sup>4</sup></u> <sup>1</sup> Advanced Light Source, Lawrence Berkeley National Laboratory <sup>2</sup> Energy Storage & Distributed Resources Division, Lawrence Berkeley National Laboratory <sup>3</sup> Materials Sciences Division, Lawrence Berkeley National Laboratory <sup>4</sup> Molecular Foundry, Lawrence Berkeley National Laboratory
11:40-11:50		<b>Comparison of resonant and non-resonant reporter for the selection of brightest gold nanoparticles for Surface-enhanced Raman spectroscopy.</b> <u>Megha Mehta<sup>1</sup>, William Skinner<sup>1</sup>, Sara Mosca<sup>2</sup>, Benjamin Gardner<sup>1</sup>, Francesca Palombo<sup>1</sup>, Pavel Matousek<sup>2</sup>, Nicholas Stone<sup>1</sup></u> <sup>1</sup> University of Exeter <sup>2</sup> STFC Rutherford Appleton Laboratory
	A0-04	<b>(F) Advances in instrumentation</b> Chair: Kerstin Ramser
10:45-11:00		<b>Comparison of ATR-FTIR and O-PTIR techniques at ISMI beamline for the characterisation of biological and cultural heritage samples</b> <u>Krzysztof Banas<sup>1</sup>, Agnieszka Banas<sup>1</sup>, Mark Breese<sup>1</sup></u> <sup>1</sup> Singapore Synchrotron Light Source
11:05-11:20		<b>Emerging Trend in AFM-IR: Surface-sensitive mode to probe sample's very surface</b> <u>Ariane Deniset-Besseau<sup>1</sup>, Jérémie Mathurin<sup>2</sup>, Alexandre Dazzi<sup>1</sup></u> <sup>1</sup> Institut de Chimie-Physique, Université Paris-Saclay <sup>2</sup> Institut de Chimie-Physique, CNRS



11:25-11:35		<b>SR-FTIR Imaging of Live Cells Using a Novel Demountable Flow System to Study Phospholipidosis</b> Ohood Alshareef <sup>1</sup> , K.L Andrew Chan <sup>1</sup> , Ben Forbes <sup>1</sup> , Mohamed Alhnan <sup>1</sup> , Gianfelice Cinque <sup>2</sup> <sup>1</sup> Institute of Pharmaceutical Sciences, King's College London <sup>2</sup> Diamond Light Source, Harwell Science and Innovation Campus
11:40-11:50		<b>Infrared spectroscopy at the user facility ELI Beamlines</b> Nils Lenngren <sup>1</sup> , Mateusz Rebarz <sup>1</sup> , Jakob Andreasson <sup>1</sup> , Miroslav Klotz <sup>1</sup> <sup>1</sup> The Extreme Light Infrastructure ERIC
11:55-12:05		<b>Current status of Chemical Infrared Imaging (CIRI / SOLAIR) beamline in Solaris</b> Maciej Roman <sup>1</sup> , Danuta Liberda <sup>1</sup> , Paulina Koziol <sup>1</sup> , Karolina Kosowska <sup>1</sup> , Tomasz P. Wrobel <sup>1</sup> <sup>1</sup> SOLARIS National Synchrotron Radiation Centre, Jagiellonian University
	A0-03	<b>(G) Analytical applications</b> Chair: Young Mee Jung
10:45-11:00		<b>SERS combined with chemometric analysis for detection and identification of microorganisms: viruses and bacteria.</b> Agnieszka Kamińska <sup>1</sup> , Krzysztof Niciński <sup>1</sup> , Sylwia Berus <sup>1</sup> , Dorota Korsak <sup>2</sup> , Tomasz Szymborski <sup>1</sup> , Beata Młynarczyk-Bonikowska <sup>3</sup> , Monika Adamczyk-Popławska <sup>2</sup> , Evelin Witkowska <sup>1</sup> <sup>1</sup> Institute of Physical Chemistry, Polish Academy of Sciences <sup>2</sup> University of Warsaw, Faculty of Biology, Institute of Microbiology <sup>3</sup> Department of Dermatology and Venerology, Medical University of Warsaw
11:05-11:20		<b>SISSI-Bio: the multipurpose infrared laboratory at Elettra synchrotron facility</b> Lisa Vaccari <sup>1</sup> , Giovanni Birarda <sup>1</sup> , Federica Piccirilli <sup>1</sup> , Diana Eva Bedolla <sup>2</sup> , Chiaramaria Stani <sup>3</sup> <sup>1</sup> Elettra Sincrotrone Trieste <sup>2</sup> Area Science Park <sup>3</sup> CERIC-ERIC
11:25-11:35		<b>SERS-based detection schemes in complex biological matrices</b> Dana Cialla-May <sup>1</sup> , Natalia E. Markina <sup>2</sup> , Alexey V. Markin <sup>2</sup> , Juergen Popp <sup>1</sup> <sup>1</sup> Leibniz Institute of Photonic Technology <sup>2</sup> Saratov State University
11:40-11:50		<b>Quantitative Raman Analysis of Carotenoid Protein Complexes in Aqueous Solution</b> Joy Udensi <sup>1</sup> , Ekaterina Loskutova <sup>1</sup> , James Loughman <sup>1</sup> , Hugh Byrne <sup>1</sup> <sup>1</sup> Technological University Dublin
11:55-12:05		<b>Towards a SERS electronic nose: VOC and gas sensing</b> Elle Wyatt <sup>1</sup> , Marika Niihori <sup>1</sup> , Sarah Sibug-Torres <sup>1</sup> , Rakesh Arul <sup>1</sup> , David- Benjamin Grys <sup>1</sup> , Bart De Nijs <sup>1</sup> , Jeremy Baumberg <sup>1</sup> <sup>1</sup> University of Cambridge
12:10-13:10		<b>Lunch</b>
13:10-14:35		<b>SESSION 2</b>
	A1-01	<b>(B) Structure &amp; dynamics of molecules</b> Chair: Federica Piccirilli
13:10-13:25		<b>Electrostatic and electrodynamic fields in lipid bilayer membranes</b> Lauren Webb <sup>1</sup> <sup>1</sup> The University of Texas at Austin
13:30-13:45		<b>Probing protein structure on nanoparticle surfaces using theoretical and experimental sum frequency scattering spectroscopy</b> Tobias Weidner <sup>1</sup> <sup>1</sup> Department of Chemistry, Aarhus University, Denmark, email: weidner@chem.au.dk
13:50-14:00		<b>FTIR studies of mutual interaction in PLL-doped DPPC/DPPG membranes: a powerful insight by chemometric analysis</b> Paulina Trombik <sup>1</sup> , Mirosław Czarnecki <sup>1</sup> , Katarzyna Cieślík-Boczula <sup>1</sup> <sup>1</sup> Faculty of Chemistry, University of Wrocław, F. Joliot-Curie 14, 50-383 Wrocław
14:05-14:15		<b>Crystalline purines in microalgae: Surprising robustness of the biosynthesis of crystalline guanine in dinoflagellates</b> Peter Mojžeš <sup>1</sup> , Maxim Bokov <sup>1</sup> , Radek Bura <sup>1</sup> , Jana Pilátová <sup>2</sup> <sup>1</sup> Charles University, Faculty of Mathematics and Physics, Institute of Physics <sup>2</sup> Charles University, Faculty of Science, Department of Experimental Plant Biology

	A1-02	<b>(C) Spectroscopy in local fields</b> Chair: Agata Królikowska
13:10-13:25		<b>Surface-Enhanced Anti-Stokes Intensity Fluctuations at High Speed</b> <u>Alexandre Brolo</u> <sup>1</sup> , Nathan Lindquist <sup>2</sup> <sup>1</sup> University of Victoria <sup>2</sup> Bethel University
13:30-13:45		<b>Spectrally Resolved Super-Resolution Surface Enhanced Raman Scattering Imaging</b> <u>Zachary Schultz</u> <sup>1</sup> <sup>1</sup> The Ohio State University
13:50-14:00		<b>Beyond the metal core: leveraging stabilizer-metal interactions for direct SERS detection</b> Chiara Deriu <sup>1</sup> , Laura Fabris <sup>1</sup> <sup>1</sup> Politecnico di Torino
14:05-14:15		<b>Exploring and Optimizing Factors Influencing Surface-Enhanced Raman Scattering (SERS) Performance</b> <u>Sylwester Gawinkowski</u> <sup>1</sup> <sup>1</sup> Institute of Physical Chemistry, Polish Academy of Sciences
14:20-14:30		<b>In vivo Real-time Multiplex Detection of Plant Signalling Molecules Using Surface-Enhanced Raman Scattering Nanosensor</b> <u>Won Ki Son</u> <sup>1</sup> <sup>1</sup> Seoul National University
	A0-04	<b>(F) Advances in instrumentation</b> Chair: Agnieszka Banas
13:10-13:20		<b>Dxcover® Platform: The next generation of ATR-FTIR spectroscopy</b> <u>Holly Butler</u> <sup>1</sup> , Loren Christie <sup>1</sup> , Matthew J. Baker <sup>2</sup> <sup>1</sup> Dxcover Ltd <sup>2</sup> School of Medicine, University of Central Lancashire
13:25-13:35		<b>Infrared nanoimaging and nanospectroscopy – emerging tools for physical and (bio)chemical nanoanalytics</b> <u>Adrian Cernescu</u> <sup>1</sup> <sup>1</sup> attocube systems AG
13:40-13:50		<b>Most recent advances of QCL-IR microspectroscopy</b> <u>Matthias Godejohann</u> <sup>1</sup> <sup>1</sup> MG Optical Solutions
13:55-14:05		<b>Widefield Super-Resolution IR Imaging with Fluorescence Enhanced Photothermal Infrared</b> <u>Miriam Unger</u> <sup>1</sup> , Mustafa Kansiz <sup>1</sup> <sup>1</sup> Photothermal Spectroscopy Corp
14:10-14:20		<b>Nano-Sized and Wearable Raman Spectrometers: Towards Widespread of SERs and Vibrational Spectroscopy</b> <u>William Terziyan</u> <sup>1</sup> , Daniel Lauriola <sup>1</sup> , Chase Wang <sup>1</sup> <sup>1</sup> BaySpec, Inc.
	A0-03	<b>(G) Analytical applications</b> Chair: Yaakov Tischler
13:10-13:20		<b>Correlation analysis of spectroscopic and biological features to follow mesenchymal stem cell differentiation</b> <u>Karolina Augustyniak</u> <sup>1</sup> , Hubert Latka <sup>1</sup> , Monika Lesniak <sup>2</sup> , Jacek Z. Kubiak <sup>2</sup> , Robert Zdanowski <sup>2</sup> , Kamilla Malek <sup>1</sup> <sup>1</sup> Jagiellonian University, Department of Chemical Physics <sup>2</sup> Military Institute of Medicine – National Research Institute, Laboratory of Molecular Oncology and Innovative Therapies
13:25-13:35		<b>Thriving Advantages of Drug Combination in Osteosarcoma Treatment – A Vibrational Microspectroscopy Study</b> <u>Raquel C. Laginha</u> <sup>1</sup> , <u>Jéssica D. Silva</u> <sup>1</sup> , <u>Maria Paula M. Marques</u> <sup>1</sup> , <u>Gianfelice Cinque</u> <sup>2</sup> , <u>Luís A. E. Batista de Carvalho</u> <sup>1</sup> , <u>Ana L.M. Batista de Carvalho</u> <sup>1</sup> <sup>1</sup> Molecular Physical-Chemistry R&D Unit <sup>2</sup> Diamond Light Source

13:40-13:50		<b>ATR-FTIR spectroscopic study of cells from the human monocytic cell line MONO-MAC-6 with stimulation by insulin</b> H. Michael Heise <sup>1</sup> , Jacinta Tomas Borges <sup>1</sup> , Yannik Merx <sup>1</sup> , Saskia Simon <sup>1</sup> , Sandra Stoppelkamp <sup>1</sup> <sup>1</sup> SOUTH-WESTPHALIA UNIVERSITY OF APPLIED SCIENCES
13:55-14:05		<b>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</b> Valentina Notarstefano <sup>1</sup> , Alessia Belloni <sup>1</sup> , Paolo Mariani <sup>1</sup> , Elisabetta Giorgini <sup>1</sup> , Hugh J. Byrne <sup>2</sup> <sup>1</sup> Marche Polytechnic University <sup>2</sup> Technological University Dublin
14:10-14:20		<b>Multimodal Spectroscopic Imaging (MALDI MSI vs Raman imaging / FTIR ) in the analysis of the secondary metabolites</b> Mikolaj Krysa <sup>1</sup> , Katarzyna Suśniak <sup>2</sup> , Monika Szymańska-Chargot <sup>3</sup> , Anna Sroka-Bartnicka <sup>1</sup> <sup>1</sup> Independent Unit of Spectroscopy and Chemical Imaging, Biomedical Faculty, Medical University of Lublin <sup>2</sup> 1Independent Unit of Spectroscopy and Chemical Imaging, Biomedical Faculty, Medical University of Lublin; 2 Department of Genetics and Microbiology, Institute of Biological Sciences, Maria Curie-Skłodowska University <sup>3</sup> Institute of Agrophysics, Polish Academy of Sciences
14:25-14:35		<b>Spectroscopic analysis of cancer-derived small extracellular vesicles for in vitro cancer diagnosis</b> Yuling Wang <sup>1</sup> , Wei Zhang <sup>1</sup> <sup>1</sup> Macquarie University
14:30-15:00		<b>Coffee Break</b>
15:00-16:15		<b>SESSION 3</b>
	A1-01	<b>(B) Structure&amp;dynamics of molecules</b> Chair: Piotr Mak
15:00-15:10		<b>In-cell IR Difference Spectroscopy as a Time-resolved Method to Study Proteins in Living Cells</b> Lukas Goett-Zink <sup>1</sup> , Anna Toschke <sup>1</sup> , Eileen Baum <sup>1</sup> , Tilman Kottke <sup>1</sup> <sup>1</sup> Bielefeld University / Biophysical Chemistry and Diagnostics
15:15-15:25		<b>Nanosecond time-resolved IR spectroscopy on proteins using quantum cascade laser setups</b> Jessica Klocke <sup>1</sup> , Tilman Kottke <sup>1</sup> <sup>1</sup> Biophysical Chemistry and Diagnostics, Bielefeld University
15:30-15:40		<b>Rapidly determining the 3D structure of proteins by Surface-enhanced Raman spectroscopy</b> Hao Ma <sup>1</sup> , Bin Ren <sup>1</sup> <sup>1</sup> Xiamen University
15:45-15:55		<b>Decoding early signs of erythrocyte pathology through analysis of protein secondary structure alterations</b> Tetiana Stepanenko <sup>1</sup> , Katarzyna Bułat <sup>2</sup> , Natalia Wilkosz <sup>2</sup> , Fatih C. Alcicek <sup>3</sup> , Jakub Dybas <sup>4</sup> , Katarzyna M. Marzec <sup>5</sup> <sup>1</sup> Jagiellonian University, National Synchrotron Radiation Centre SOLARIS <sup>2</sup> Łukasiewicz Research Network, Krakow Institute of Technology <sup>3</sup> Goethe University, Institute for Cardiovascular Physiology <sup>4</sup> Jagiellonian University, Jagiellonian Centre for Experimental Therapeutics (JCET) <sup>5</sup> AGH University of Science and Technology, Faculty of Physics and Applied Computer Science, Department of Medical Physics and Biophysics
16:00-16:10		<b>Hydration Structure of Biomaterials Studied by Infrared Spectroscopy and Chemometrics</b> Shigeaki Morita <sup>1</sup> <sup>1</sup> Osaka Electro-Communication University
	A1-02	<b>(C) Spectroscopy in local fields</b> Chair: Zachary Schultz
15:00-15:15		<b>In-situ study of nanocatalytic reactions using surface-enhanced Raman spectroscopy</b> Hua Zhang <sup>1</sup> <sup>1</sup> College of Materials Xiamen University"
15:20-15:35		<b>Precision reusable flow SERS for Healthcare BioSensors 2.0</b> Jeremy Baumberg <sup>1</sup> <sup>1</sup> University of Cambridge

15:40-15:50		<b>Exciton-Phonon Coupling in MoSe<sub>2</sub>/WSe<sub>2</sub> Heterobilayers Probed Using Resonant Raman Spectroscopy</b> Oisín Garrity <sup>1</sup> , Thomas Brumme <sup>2</sup> , Annika Bergmann <sup>3</sup> , Tobias Korn <sup>3</sup> , Patryk Kusch <sup>1</sup> , Stephanie Reich <sup>1</sup> <sup>1</sup> Freie Universität Berlin <sup>2</sup> Technische Universität Dresden <sup>3</sup> Universität Rostock
15:55-16:05		<b>In-Situ Cost-effective Methods for Fabricating SERS Substrates using Polydopamine</b> Ahmed Mahmoud <sup>1</sup> , Alexandra Teixeira <sup>1</sup> , Maria Sousa-Silva <sup>1</sup> , Sara Abalde-Cela <sup>1</sup> , Lorena Diéguez <sup>1</sup> <sup>1</sup> The International Iberian Nanotechnology Laboratory (INL)
16:10-16:20		<b>Vanadium oxide nanoparticles as non-plasmonic platforms for surface-enhanced Raman spectroscopy</b> Eva Kočíšová <sup>1</sup> , Anna Kuzminova <sup>2</sup> , Marek Procházka <sup>1</sup> , Ondřej Kylián <sup>2</sup> <sup>1</sup> Institute of Physics, Faculty of Mathematics and Physics, Charles University <sup>2</sup> Department of Macromolecular Physics, Faculty of Mathematics and Physics, Charles University
	A0-04	<b>(F) Advances in instrumentation</b> Chair: Holly Butler
15:00-15:15		<b>Through the looking glass: Raman imaging through the bottle</b> Kishan Dholakia <sup>1</sup> <sup>1</sup> University of Adelaide
15:20-15:35		<b>New Approaches for Raman Spectroscopic Imaging and High-Throughput Monitoring in Biomedical Applications</b> Torsten Frosch <sup>1</sup> <sup>1</sup> Technical University Darmstadt
15:40-15:50		<b>Mode Optimized Tip-Enhanced Raman Scattering</b> Tao Chen <sup>1</sup> , Wei Wang <sup>1</sup> , Volker Deckert <sup>1</sup> <sup>1</sup> Friedrich-Schiller University
15:55-16:05		<b>Electric-field-dependent infrared nanospectroscopy of PVDF with an atomic force microscope</b> Maria Eleonora Temperini <sup>1</sup> , Valeria Giliberti <sup>2</sup> , Tommaso Venanzi <sup>2</sup> , Raffaella Polito <sup>1</sup> , Antonia Intze <sup>1</sup> , Michele Ortolan <sup>1</sup> <sup>1</sup> Sapienza University of Rome
16:10-16:20		<b>Detection of microplastics using optical manipulation techniques and Raman spectroscopy</b> Silvie Bernatová <sup>1</sup> , Martin Kizovský <sup>1</sup> , Antonino Foti <sup>2</sup> , Maria Donato <sup>2</sup> , Pavel Zemánek <sup>1</sup> , Ota Samek <sup>1</sup> , Onofrio Maragò <sup>2</sup> , Jan Ježek <sup>1</sup> , Pietro Gucciardi <sup>2</sup> <sup>1</sup> Institute of Scientific Instruments of the Czech Academy of Sciences <sup>2</sup> Istituto per Processi Chimico-Fisici – Consiglio Nazionale delle Ricerche
	A0-03	<b>(G) Analytical applications</b> Chair: Cassio Lima
15:00-15:10		<b>Chemically-specific in situ coherent Raman imaging of liquid-liquid phase separation in the crystallization process of pharmaceutical solids</b> Alba Arbiol <sup>1</sup> , Laurin Zöller <sup>2</sup> , Teemu Tomberg <sup>1</sup> , Jukka Saarinen <sup>1</sup> , Tom Konings <sup>1</sup> , Sara Carlert <sup>3</sup> , Eva Karlsson <sup>3</sup> , Anders Borde <sup>2</sup> , Quentin Vicentini <sup>2</sup> , Christoph Saal <sup>3</sup> , Jennifer Dressman <sup>2</sup> , Clare Strachan <sup>1</sup> <sup>1</sup> Division of Pharmaceutical Chemistry and Technology, Viikinkaari 5E, 00014 University of Helsinki, Finland <sup>2</sup> Fraunhofer Institute for Translational Medicine and Pharmacology ITMP, Germany <sup>3</sup> AstraZeneca R&D Mölndal, S-431 83 Mölndal, Sweden
15:15-15:25		<b>Spectral identification of therapeutic allergen products</b> Christian Ickes <sup>1</sup> , Piryá Rani <sup>2</sup> , Kristiyana Tsenova <sup>3</sup> , Johanna Rost <sup>1</sup> , Frank Führer <sup>1</sup> , Detlef Bartel <sup>1</sup> , Christel Kamp <sup>1</sup> <sup>1</sup> Paul-Ehrlich-Institut <sup>2</sup> Saarland University <sup>3</sup> Goethe University

15:30-15:40		<b>Raman-based Detection of Antibiotics and Metabolites in Pharmaceutical Formulations and Clinical-relevant Matrices</b> Chen Liu <sup>1</sup> , Jürgen Popp <sup>1</sup> , Dana Cialla-May <sup>2</sup> <sup>1</sup> Institute of Physical Chemistry (IPC) and Abbe Center of Photonics (ACP), Friedrich Schiller University Jena, Member of the Leibniz Centre for Photonics in Infection Research (LPI), Helmholtzweg 4, 07743 Jena, Germany <sup>2</sup> Leibniz Institute of Photonic Technology, Member of Leibniz Health Technologies, Member of the Leibniz Centre for Photonics in Infection Research (LPI), Albert-Einstein-Straße 9, 07745 Jena, Germany
15:45-15:55		<b>Insights into triglycerides removal: Study using FTIR and Raman imaging in flow and static conditions</b> Gunjan Tyagi <sup>1</sup> , Zain Ahmed <sup>1</sup> , Joao Cabral <sup>1</sup> , Sergei Kazarian <sup>1</sup> <sup>1</sup> Imperial College London
16:05-16:15		<b>Rare earth-citrate complexes study using surface-enhanced Raman scattering spectra</b> Hao Jin <sup>1</sup> , Tamitake Itoh <sup>2</sup> , Yuko. S. Yamamoto <sup>1</sup> <sup>1</sup> School of Materials Science, Japan Advanced Institute of Science and Technology <sup>2</sup> Nano-Bioanalysis Research Group, Health Research Institute, National Institute of Advanced Industrial Science and Technology
16:30-18:45		<b>POSTER SESSION 1</b>
		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		<b>Steering Committee meeting</b>
<b>Tuesday</b>		
9:00-10:15	A0-01	<b>Plenary Session</b>
		Chair: Gulietta Smulevich
9:00-9:30		<b>What we learn with new time-resolved Raman spectrometers</b> Koichi Iwata <sup>1</sup> <sup>1</sup> Gakushuin University
		Chair: Yukihiko Ozaki
9:40-10:10		<b>Ultrafast Structural Dynamics in Various <math>\pi</math>-Conjugated Molecular Systems Probed by Time-resolved Electronic and Vibrational Spectroscopy</b> Dongho Kim <sup>1</sup> <sup>1</sup> Department of Chemistry, Yonsei University
10:15-10:45		<b>Coffe Break</b>
10:45-12:10		<b>SESSION 1</b>
	A1-01	<b>(B) Structure&amp;dynamics of molecules</b> Chair: Valeria Giliberti
10:45-11:00		<b>Domain movements and conformational changes in large membrane proteins identified by combined SEIRAS and IR labelling approach</b> Petra Hellwig <sup>1</sup> , Tatjana Gerasimova <sup>2</sup> , Ana Filipa Seica Santos <sup>3</sup> , Thorsten Friedrich <sup>4</sup> <sup>1</sup> University of Strasbourg CNRS, UMR 7140 <sup>2</sup> University of Strasbourg and University of Freiburg <sup>3</sup> University of Strasbourg, UMR 7140 <sup>4</sup> University of Freiburg, Institute for Biochemistry
11:05-11:20		<b>Local Structural Dynamics of Membrane Protein Bacteriorhodopsin Revealed by 2D Vibrational Spectroscopy</b> Jianping Wang <sup>1</sup> <sup>1</sup> Institute of Chemistry
11:25-11:35		<b>Plasmonic infrared study of SARS COV-2 mPro dimerization and its inibition</b> Federica Piccirilli <sup>1</sup> , Giovanni Birarda <sup>1</sup> , Lisa Vaccari <sup>1</sup> , Hendrik Vondracek <sup>1</sup> , Lucia Silvestini <sup>2</sup> , Francesco Spinozzi <sup>3</sup> , Paolo Mariani <sup>3</sup> , Antonio Palumbo Piccionello <sup>4</sup> , Vincenzo Aglieri <sup>5</sup> , Andrea Toma <sup>5</sup> , Maria Grazia Ortore <sup>3</sup> <sup>1</sup> Elettra Sincrotrone Trieste <sup>2</sup> Università politecnica delle Marche <sup>3</sup> Università Politecnica delle Marche <sup>4</sup> Università degli studi di Palermo <sup>5</sup> Istituto Italiano di tecnologia



11:40-11:50		<b>The chemical structure and conformation of tau protein aggregates at the growth phase</b> Kamila Sofińska <sup>1</sup> , Sara Seweryn <sup>1</sup> , Katarzyna Skirlińska-Nosek <sup>1</sup> , Piotr Batys <sup>2</sup> , Jakub Barbasz <sup>2</sup> , Ewelina Lipiec <sup>1</sup> <sup>1</sup> Jagiellonian University, Faculty of Physics, Astronomy, and Applied Computer Science, M. Smoluchowski Institute of Physics <sup>2</sup> Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences
	A1-02	<b>(C) Spectroscopy in local fields</b> Chair: Eva Kočíšová
10:45-11:00		<b>Studying Metal-Molecule Interactions to Improve SERS Sensor Performance</b> Laura Fabris <sup>1</sup> , Chiara Deriu <sup>1</sup> , Kaleigh Scher <sup>2</sup> , Shaila Thakur <sup>1</sup> <sup>1</sup> Politecnico di Torino <sup>2</sup> Rutgers University
11:05-11:20		<b>Comparative study of p-Aminothiophenol adsorption by Surface-Enhanced Raman Spectroscopy</b> María Rosa López-Ramírez <sup>1</sup> , María De la Cabeza Fernández <sup>2</sup> , Alexis Alvear-Fernández <sup>2</sup> , Rafael Contreras-Cáceres <sup>3</sup> <sup>1</sup> Department of Physical Chemistry, Faculty of Science, University of Málaga <sup>2</sup> Department of Chemistry in Pharmaceutical Sciences, Faculty of Pharmacy, Universidad Complutense de Madrid <sup>3</sup> Department of Chemistry and Physics, University of Almería
11:25-11:35		<b>Searching for one-armed thiol bandit – SERS and DFT studies on adsorption modes of cyclo(L-Cys-D-Cys) on silver</b> Agata Królikowska <sup>1</sup> , Marcin Witkowski <sup>1</sup> , Lasse Jensen <sup>2</sup> , Wojciech Dzwolak <sup>1</sup> <sup>1</sup> Faculty of Chemistry, University of Warsaw, Pasteura 1 <sup>2</sup> Department of Chemistry, Penn State University, 101 Chemistry Building, University Park, 16802, PA
11:40-11:50		<b>A newly recognized chemically stable surface bound thiolate intermediate in plasmon-induced catalysis</b> Xiaobin Yao <sup>1</sup> , Sadaf Ehtesabi <sup>2</sup> , Christiane Höppener <sup>1</sup> , Tanja Deckert-Gaudig <sup>1</sup> , Henrik Schneidewind <sup>3</sup> , Stephan Kupfer <sup>2</sup> , Stefanie Gräfe <sup>2</sup> , Volker Deckert <sup>1</sup> <sup>1</sup> 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 <sup>2</sup> 1. Friedrich Schiller University Jena, Institute of Physical Chemistry and Abbe Center of Photonics, Helmholtzweg 4, Jena 07743, Germany <sup>3</sup> 2. Leibniz Institute of Photonic Technology, Albert-Einstein-Str.9, Jena 07745, Germany
11:55-12:05		<b>Pushing the limits of Raman Spectroscopy: Photo-induced enhanced Raman Spectroscopy on Ag-TiO<sub>2</sub> hybrid nanoplatfoms</b> Łukasz Pięta <sup>1</sup> , Aneta Kisielewska <sup>2</sup> , Ireneusz Piwoński <sup>2</sup> , Kamilla Małek <sup>1</sup> <sup>1</sup> Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Krakow, Poland <sup>2</sup> Department of Materials Technology and Chemistry, Faculty of Chemistry, University of Lodz, Pomorska 163, 90-236 Lodz, Poland
	A0-04	<b>(F) Advances in instrumentation</b> Chair: Wojciech Kwiatek
10:45-10:55		<b>Simultaneous SERS &amp; SEIRA with Single Molecule Detection – The Application and Characterization of Plasmonically Resonant Structures with Sub-Micron Optical Photothermal Infrared and Simultaneous Raman spectroscopy</b> Mustafa Kansiz <sup>1</sup> , Miriam Unger <sup>2</sup> , Deepthy Kavungal <sup>3</sup> , Felix Richter <sup>4</sup> , Hatice Altug <sup>3</sup> , Mark Anderson <sup>5</sup> <sup>1</sup> Photothermal Spectroscopy Corp <sup>2</sup> Photothermal Spectroscopy Corp GmbH <sup>3</sup> Bionanophotonic Systems (BIOS) Laboratory & Lashuel Lab, EFPL <sup>4</sup> Bionanophotonic Systems (BIOS) Laboratory & Lashuel Lab, EFPL, <sup>5</sup> Caltech, Jet Propulsion Labs, NASA
11:00-11:10		<b>Raman optical activity as a sensitive tool in analytical chemistry</b> Josef Kapitán <sup>1</sup> , Pavel Michal <sup>1</sup> , Jana Hudecová <sup>1</sup> , Petr Bouř <sup>2</sup> <sup>1</sup> Palacký University Olomouc, Department of Optics <sup>2</sup> Institute of Organic Chemistry and Biochemistry, Academy of Sciences

11:15-11:25		<b>A novel wide-field Raman imaging setup</b> B. J. A Mooij <sup>1</sup> , R. W. Schmidt <sup>1</sup> , W. A. J. Vijvers <sup>2</sup> , F. Arie <sup>1</sup> <sup>1</sup> LaserLaB, Vrije Universiteit Amsterdam <sup>2</sup> Chromodynamics B.V.
11:30-11:40		<b>Simultaneous co-located Raman and SEM imaging for correlated SEM microscopy</b> Jorge Diniz <sup>1</sup> , Agnieszka Sozanska <sup>2</sup> , Tim Batten <sup>3</sup> <sup>1</sup> Renishaw plc <sup>2</sup> Renishaw Spzoo <sup>3</sup> Renishaw PLC
11:45-11:55		<b>Reducing frequency fluctuations induced by back-reflected light into a non-stabilized low cost laser diode</b> Konstantinos Stergiou <sup>1</sup> , Oleksii Ilchenko <sup>2</sup> , Yurii Pilhun <sup>1</sup> , Andrii Kutsyk <sup>2</sup> <sup>1</sup> Lightnovo ApS <sup>2</sup> Technical University of Denmark
12:00-12:10		<b>Maximizing Positive Microplastic Particle Identification and Provenance Through Optimized Optical and Raman Microscopy – Particle-Correlated Raman Spectroscopy (PCRS)</b> Andrew Whitley <sup>1</sup> , Eunah Lee <sup>1</sup> , Massimiliano Rocchia <sup>1</sup> , Sebastien Laden <sup>1</sup> <sup>1</sup> HORIBA
	A0-03	<b>(G) Analytical applications</b> Chair: Entesar Al-Hetlani
10:45-10:55		<b>Silicon within fossil and cultivated coccoliths of <i>Helicosphaera carteri</i>: new insights from Infrared Spectromicroscopy and X-ray Fluorescence analyses</b> Giovanni Birarda <sup>1</sup> , Manuela Bordiga <sup>2</sup> , Diana Eva Bedolla <sup>3</sup> , Alessandra Gianoncelli <sup>1</sup> , Simone Pollastri <sup>1</sup> , Valentina Bonanni <sup>1</sup> , Gianluca Gariani <sup>1</sup> , Lisa Vaccari <sup>1</sup> , Federica Cerino <sup>2</sup> , Marina Cabrini <sup>2</sup> , Alfred Beran <sup>2</sup> , Mario Zanon <sup>4</sup> , Maurizio Zuccotti <sup>4</sup> , Giulia Fiorentino <sup>4</sup> , Miriam Cobianchi <sup>5</sup> , Andrea Di Giulio <sup>5</sup> , Claudia Lupi <sup>5</sup> <sup>1</sup> Elettra—Sincrotrone Trieste <sup>2</sup> National Institute of Oceanography and Applied Geophysics OGS <sup>3</sup> AREA Science Park <sup>4</sup> Department of Biology and Biotechnologies “Lazzaro Spallanzani”, University of Pavia <sup>5</sup> Department of Earth and Environmental Sciences, University of Pavia
11:00-11:10		<b>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</b> Joanna Chwiej <sup>1</sup> , Natalia Janik-Olchawa <sup>2</sup> , Agnieszka Drózd <sup>3</sup> , Aleksandra Wajda <sup>2</sup> , Maciej Sitarz <sup>1</sup> , Daniel Horak <sup>4</sup> , Michal Babic <sup>4</sup> , Jolanta Gol <sup>1</sup> , Zuzanna Setkiewicz-Janeczko <sup>2</sup> , Aleksandra Wilk <sup>1</sup> , Marzena Rugieł <sup>1</sup> , Katarzyna Matusiak <sup>1</sup> , Christoph Sandt <sup>5</sup> , Ferenc Borondics <sup>5</sup> , Magdalena Wytrwał-Sarna <sup>1</sup> <sup>1</sup> AGH University of Krakow <sup>2</sup> Jagiellonian University <sup>3</sup> Maria Curie-Skłodowska University in Lublin <sup>4</sup> Czech Academy of Sciences <sup>5</sup> SOLEIL
11:15-11:25		<b>The increase of fibres and flavonoids concentration in the Zea mays stem treated with Nod-factor-based biofertilizer. A multimodal imaging study.</b> Mikolaj Krysa <sup>1</sup> , Katarzyna Susniak <sup>2</sup> , Cai Li Song <sup>3</sup> , Monika Szymanska-Chargot <sup>4</sup> , Artur Zdunek <sup>4</sup> , Izabela S. Pieta <sup>5</sup> , Janusz Podlesny <sup>6</sup> , Anna Sroka-Barnicka <sup>1</sup> , Sergei G. Kazarian <sup>3</sup> <sup>1</sup> Medical University of Lublin, Independent Unit of Spectroscopy and Chemical Imaging, <sup>2</sup> Maria Curie-Skłodowska University, Department of Genetics and Microbiology <sup>3</sup> Imperial College London, Department of Chemical Engineering <sup>4</sup> Institute of Agrophysics, Polish Academy of Sciences <sup>5</sup> Institute of Physical Chemistry, Polish Academy of Sciences <sup>6</sup> Institute of Soil Science and Plant Cultivation, State Research Institute
11:30-11:40		<b>Development of Raman Spectroscopic analysis techniques to assess quality biomarkers in fish</b> Jeremy Landry <sup>1</sup> , Peter Torley <sup>1</sup> , Ewan Blanch <sup>1</sup> <sup>1</sup> RMIT University

11:45-11:55		<b>Visualization and identification of components in a gigantic spherical dolomite concretion by Raman imaging and MCR analysis</b> Ryosuke Kitanaka <sup>1</sup> , Motohiro Tsuboi <sup>2</sup> , Tomoko Numata <sup>3</sup> , Yusuke Muramiya <sup>4</sup> , Hidekazu Yoshida <sup>5</sup> , Yukihiro Ozaki <sup>2</sup> <sup>1</sup> Kewansei Gakuin University <sup>2</sup> Kwansei Gakuin University <sup>3</sup> HORIBA Techno Service Co. Ltd. <sup>4</sup> Fukada Geological Institute <sup>5</sup> Nagoya University
12:00-12:10		<b>SIP vibrational microspectroscopy in micro-structured chips reveals single-cell metabolic dynamics of soil microbes</b> Milda Pucetaite <sup>1</sup> , Edith C. Hammer <sup>1</sup> , Louise C. Andresen <sup>2</sup> , Sofía Gabriela Rodas Samayoa <sup>2</sup> <sup>1</sup> Department of Biology, Lund University <sup>2</sup> Department of Earth Science, University of Gothenburg
	A0-01	<b>(H) Biodiagnostic spectroscopy</b> Chair: Nick Stone
10:45-11:00		<b>High-resolution Raman imaging of &gt;300 cells from human patients affected by nine different leukemia subtypes: a global clustering approach</b> Renzo Vanna <sup>1</sup> , Andrea Masella <sup>2</sup> , Manuela Bazzarelli <sup>2</sup> , Paola Ronchi <sup>3</sup> , Aufried Lenferink <sup>4</sup> , Cristina Tresoldi <sup>3</sup> , Carlo Morasso <sup>5</sup> , Marzia Bedoni <sup>6</sup> , Dario Polli <sup>7</sup> , Fabio Ciceri <sup>3</sup> , Giulia De Poli <sup>2</sup> , Matteo Bregonzio <sup>2</sup> , Cees Otto <sup>4</sup> <sup>1</sup> Istituto di Fotonica e Nanotecnologie – Consiglio Nazionale delle Ricerche (IFN-CNR) <sup>2</sup> 3rdPlace SRL <sup>3</sup> IRCCS Ospedale San Raffaele <sup>4</sup> University of Twente <sup>5</sup> IRCCS Istituti Clinici Scientifici Maugeri <sup>6</sup> IRCCS Fondazione Don Carlo Gnocchi <sup>7</sup> Politecnico di Milano
11:05-11:20		<b>Surface Enhanced Spatially Offset Raman Spectroscopy: A Promising Optical Imaging Modality in Preclinical Cancer Imaging</b> Fay Nicolson <sup>1</sup> , Eunah Lee <sup>2</sup> , Andrew Whitely <sup>2</sup> , Bohdan Andreiuk <sup>3</sup> , Scott Rudder <sup>4</sup> , Samuel Mabbott <sup>5</sup> , Kevin Haigis <sup>1</sup> <sup>1</sup> Dana-Farber Cancer Institute <sup>2</sup> HORIBA Scientific <sup>3</sup> Dana-Farber Cancer Institute <sup>4</sup> Opto-Sigma <sup>5</sup> Texas A&M University
11:25-11:35		<b>Surface-enhanced Raman Spectroscopy in tumor detection</b> Aneta Kowalska <sup>1</sup> , Marta Czaplicka <sup>1</sup> , Ariadna Nowicka <sup>2</sup> , Tomasz Szymborski <sup>3</sup> , Izabela Chmielewska <sup>4</sup> , Wojciech Kukwa <sup>5</sup> , Agnieszka Kamińska <sup>3</sup> <sup>1</sup> Institute of Physical Chemistry Polish Academy of Sciences <sup>2</sup> Institute for materials Research and Quantum Engineering, Poznań University <sup>3</sup> Institute of Physical Chemistry, Polish Academy of Sciences <sup>4</sup> Department of Pneumology, Oncology and Allergology, Medical University of Lublin <sup>5</sup> Szpital Czerniakowski, Medical University of Warsaw
11:40-11:50		<b>FTIR Spectroscopy for Bladder Carcinoma Detection and Prediction of Grade, Invasion, and Lymph Nodes Metastases</b> Monika Kujdowicz <sup>1</sup> , David Perez-Guaita <sup>2</sup> , Piotr Chłosta <sup>3</sup> , Krzysztof Okon <sup>4</sup> , Kamilla Malek <sup>5</sup> <sup>1</sup> Department of Patomorphology, Jagiellonian University Medical College; Faculty of Chemistry, Jagiellonian University <sup>2</sup> Department of Analytical Chemistry, University of Valencia <sup>3</sup> Department of Urology, Jagiellonian University Medical College <sup>4</sup> Department of Patomorphology, Jagiellonian University Medical College <sup>5</sup> Faculty of Chemistry, Jagiellonian University

11:55-12:05		<b>Raman Spectroscopic application in cervical cancer screening</b> Rubina Shaikh <sup>1</sup> , Aoife Mc Guinness <sup>2</sup> , Alison Malkin <sup>3</sup> , John O'Leary <sup>4</sup> , Cara Martin <sup>4</sup> , Fiona Lyng <sup>2</sup> <sup>1</sup> Marie Curie Fellow 1.Centre for Radiation and Environmental Science, FOCAS Research Institute, Technological University Dublin, Ireland. 2.School of Physics & Clinical & Optometric Sciences, Central Quad, Technological University Dublin – City Campus, Gr <sup>2</sup> 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 <sup>3</sup> TU Dublin <sup>4</sup> TCD CERVIVA Molecular Pathology Laboratory, The Coombe Women and Infants University Hospital, Dublin, Ireland.5. Trinity St James Cancer Institute, Trinity College Dublin, Ireland
12:10-13:10		<b>Lunch</b>
13:15-14:30		<b>POSTER SESSION 2</b>
		<b>Poster Session (Topics A, E, F, J)</b>
14:45-18:00		<b>Excursion</b>
19:00		<b>Beer Club</b>
<b>Wednesday</b>		
9:00-10:15		<b>Plenary Session</b>
		Chair: Kathleen Gough
9:00-9:30		<b>Advances and applications in FTIR spectroscopic imaging for studies of dynamic systems</b> Sergei Kazarian <sup>1</sup> <sup>1</sup> Imperial College London
		Chair: Christian Huck
9:40-10:10		<b>IR-control of ultrafast excited state dynamics in transition metal complexes</b> Topic: plenary and perspective lectures Julia Weinstein <sup>1</sup> , Iona Ivalo <sup>1</sup> , Rory Cowin <sup>1</sup> , Martin Appleby <sup>1</sup> , Catherine Royle <sup>1</sup> , Igor Sazanovich <sup>2</sup> , Dimitri Chekulaev <sup>3</sup> , Anthony Meijer <sup>1</sup> , Alexander Auty <sup>1</sup> , Guaznhi Wu <sup>1</sup> , Tao Cheng <sup>1</sup> , James Shipp <sup>1</sup> <sup>1</sup> University of Sheffield <sup>2</sup> Central Laser Facility, Rutherford Appleton Laboratory <sup>3</sup> Lord Porter Laser Laboratory, University of Sheffield
10:15-10:45		<b>Coffee Break</b>
10:45-12:10		<b>SESSION 1</b>
	A1-01	<b>(B) Structure&amp;dynamics of molecules</b> Chair: Judith Mihály
10:45-10:55		<b>Raman Spectroscopic Investigations of the Mechanisms of Inhibition of Protein Fibrils by Novel Spirooxindole Compounds</b> Anthony Dahdah <sup>1</sup> , Subashani Maniam <sup>1</sup> , Nilamuni De Silva <sup>1</sup> , Helmut Huegel <sup>1</sup> , Ewan Blanch <sup>1</sup> <sup>1</sup> RMIT University
11:00-11:10		<b>State of water in various environments: aliphatic ketones. MIR/NIR spectroscopic, dielectric and theoretical studies</b> Mirosław Czarnecki <sup>1</sup> , Krzysztof Beć <sup>2</sup> , Justyna Grabska <sup>2</sup> , Christian Huck <sup>2</sup> , Sylwester Mazurek <sup>1</sup> , Kazimierz Orzechowski <sup>1</sup> <sup>1</sup> University of Wrocław <sup>2</sup> University of Innsbruck
11:15-11:25		<b>Near-Infrared and visible excited Raman optical activity in the study of B12 derivatives: far-from-resonance vs strong resonance approach</b> Ewa Machalska <sup>1</sup> , Grzegorz Zając <sup>1</sup> , Monika Halat <sup>2</sup> , Takumi Tani <sup>3</sup> , Tomotsumi Fujisawa <sup>3</sup> , Masashi Unno <sup>3</sup> , Malgorzata Baranska <sup>1</sup> <sup>1</sup> Jagiellonian Centre for Experimental Therapeutics (JCET), Jagiellonian University <sup>2</sup> Department of Plant Biology and Biotechnology, Faculty of Biotechnology and Horticulture, University of Agriculture <sup>3</sup> Department of Chemistry and Applied Chemistry, Faculty of Science and Engineering, Saga University

11:30-11:40		<b>Evaluating the acidity levels in super-acidic ionic liquids by Raman Spectroscopy</b> Cedric Malherbe <sup>1</sup> <sup>1</sup> University of Liege
11:45-11:55		<b>Unraveling the Structural Polymorphism of Mononucleotide G-Quadruplexes via Raman Optical Activity</b> Štěpán Jílek <sup>1</sup> , Josef Kapitán <sup>2</sup> , Mohammed Siddique Para Kkadan <sup>1</sup> , Ivan Barvík <sup>1</sup> , Václav Profant <sup>1</sup> <sup>1</sup> Institute of Physics, Faculty of Mathematics and Physics, Charles University <sup>2</sup> Department of Optics, Faculty of Science, Palacký University Olomouc
	A1-02	<b>(E) Nonlinear vibrational spectroscopy</b> Chair: Freek Ariese
10:45-11:00		<b>Proteins at charged biointerfaces as revealed by nonlinear vibrational spectroscopy</b> Zsuzsanna Heiner <sup>1</sup> <sup>1</sup> Humboldt-Universität zu Berlin, SALSA
11:05-11:20		<b>Time-domain Raman spectroscopy for large-scale cell screening</b> Kotaro Hiramatsu <sup>1</sup> <sup>1</sup> The University of Tokyo
11:25-11:35		<b>Good vibrations: small molecule raman optical probes to image metabolism in tissue micro-environments</b> Ailsa Geddis <sup>1</sup> , Fabio De Moliner <sup>1</sup> , Colin Campbell <sup>1</sup> , Marc Vendrell <sup>1</sup> <sup>1</sup> University of Edinburgh
11:40-11:50		<b>Probing amide I-water vibrational coupling in <math>\alpha</math>-helical and <math>\beta</math>-strand protein structures with two-color two-dimensional infrared spectroscopy</b> Fani Madzharova <sup>1</sup> , Adam Chatterley <sup>1</sup> , Steven Roeters <sup>1</sup> , Tobias Weidner <sup>1</sup> <sup>1</sup> Aarhus University
11:55-12:05		<b>Molecular structure, surface charge and dissolution of the MgO-water interface influenced by liquid flow</b> Moritz Zelenka <sup>1</sup> , Ellen H. G. Backus <sup>1</sup> <sup>1</sup> University of Vienna
	A0-04	<b>(F) Advances in instrumentation</b> Chair: Yusuke Morisawa
10:45-11:00		<b>New Perspectives for Mid-IR Spectroscopy of Liquids as Enabled by Quantum Cascade Lasers</b> Bernhard Lendl <sup>1</sup> , Alicja Dabrowska <sup>1</sup> , Daniel-ralph Hermann <sup>1</sup> , Giovanna Ricchiuti <sup>1</sup> , Gustavo Lukasiwicz <sup>1</sup> , Georg Ramer <sup>1</sup> <sup>1</sup> TU Wien
11:05-11:20		<b>Stimulated Raman scattering and resonance Raman spectroscopy combined with holography, interferometry and video imaging</b> Kerstin Ramser <sup>1</sup> <sup>1</sup> Department of Engineering Sciences and Mathematics/Luleå University of Technology
11:25-11:35		<b>Developing Sensitive Stimulated Raman Scattering (SRS) Microscopy</b> Krzysztof Brzozowski <sup>1</sup> , Anna Pieczara <sup>2</sup> , Malgorzata Baranska <sup>3</sup> <sup>1</sup> Jagiellonian University <sup>2</sup> Jagiellonian Centre for Experimental Therapeutics <sup>3</sup> Jagiellonian University, Jagiellonian Centre for Experimental Therapeutics
11:40-11:50		<b>Rapid field-resolved infrared fingerprinting and discrimination of particles in flow</b> Marinus Huber <sup>1</sup> , Daniel Gerz <sup>1</sup> , Holger Mirkes <sup>2</sup> , Florian Lindinger <sup>2</sup> , Yannick Münzenmaier <sup>2</sup> , Alexander Weigel <sup>3</sup> , Mark Kielpinski <sup>1</sup> , Thomas Henkel <sup>1</sup> , Mihaela Zigman <sup>3</sup> , Ferenc Krausz <sup>3</sup> , Jürgen Popp <sup>1</sup> , Ioachim Pupeza <sup>1</sup> <sup>1</sup> Leibniz Institute of Photonic Technology <sup>2</sup> Ludwig Maximilians University <sup>3</sup> Max Planck Institute of Quantum Optics
11:55-12:05		<b>Current state of spectrometer miniaturization: synergy with analytical potential of NIR spectroscopy</b> Christian W. Huck <sup>1</sup> , Justyna Grabska <sup>1</sup> , Krzysztof B. Bec <sup>1</sup> <sup>1</sup> University of Innsbruck



	A0-03	<b>(G) Analytical applications</b> Chair: Maria Lopez-Ramirez
10:45-11:00		<b>Probing chemical speciation with low-frequency Raman spectroscopy</b> <u>Keith Gordon</u> <sup>1</sup> <sup>1</sup> University of Otago and Dodd Walls Centre – Te Whai Ao
11:05-11:20		<b>Profiling of Human Bones by Vibrational Spectroscopy</b> Maria Paula Marques <sup>1</sup> , David Gonçalves <sup>2</sup> , Stewart F. Parker <sup>3</sup> , Winfried Kockelmann <sup>3</sup> , Giulia Festa <sup>4</sup> , Luís Batista de Carvalho <sup>1</sup> <sup>1</sup> Univ. Coimbra, Molecular Physical-Chemistry R&D Unit <sup>2</sup> Archaeosciences Lab., Directorate General Cultural Heritage <sup>3</sup> ISIS Facility, STFC Rutherford Appleton Laboratory <sup>4</sup> CREF – Museo Storico della Fisica e Centro Studi e Ricerche Enrico Fermi
11:25-11:35		<b>Fusion of IR and RS spectral data in 2D and 3D in vitro studies for the spheroid blood-brain barrier model</b> Anna Antolak <sup>1</sup> , Aleksandra Pragna <sup>2</sup> , Zuzanna Krysiak <sup>3</sup> , Monika Leśniak <sup>3</sup> , Joanna Korszun <sup>4</sup> , Robert Zdanowski <sup>3</sup> , Kamilla Małek <sup>1</sup> <sup>1</sup> Jagiellonian University <sup>2</sup> Jagiellonian University, Doctoral School of Exact and Natural Sciences <sup>3</sup> Military Institute of Medicine National Research Institute <sup>4</sup> Military Institute of Medicine National Research Institute; Bio-Med-Chem Doctoral School of the University of Lodz and Lodz Institute of the Polish Academy of Sciences
11:40-11:50		<b>Aging in coronal dentine of the human tooth seen at the sub-micron resolution in non-contact IR spectroscopy</b> <u>Agnieszka Banas</u> <sup>1</sup> , Krzysztof Banas <sup>1</sup> , Chin-ying, Stephen Hsu <sup>2</sup> , Guang Rong Tang <sup>2</sup> , Mark B.H. Breese <sup>1</sup> <sup>1</sup> Singapore Synchrotron Light Source NUS <sup>2</sup> National University of Singapore, Dentistry Department
11:55-12:05		<b>Micro and nano-spectroscopic studies of modified metallic surface for implantology application</b> <u>Dominika Świąch</u> <sup>1</sup> , Gaetano Palumbo <sup>1</sup> , Natalia Piergies <sup>2</sup> , Kamila Kollbek <sup>3</sup> , Czesława Paluszkiwicz <sup>2</sup> <sup>1</sup> AGH University of Science and Technology, Faculty of Foundry Engineering, av. Mickiewicza 30 <sup>2</sup> Institute of Nuclear Physics Polish Academy of Sciences <sup>3</sup> AGH University of Science and Technology, Academic Centre for Materials and Nanotechnology, av. Mickiewicza 30
	A0-01	<b>(H) Biodiagnostic spectroscopy</b> Chair: Anna Sroka-Bartnicka
10:45-11:00		<b>Portable Raman spectroscopy for in-clinic skin and prostate cancer diagnosis</b> Suse J. Van Breugel <sup>1</sup> , Hannah Matthews <sup>1</sup> , Kamran Zargar-Shoshtari <sup>2</sup> , Paul Jarret <sup>3</sup> , Michelle Locke <sup>4</sup> , Cather Simpson <sup>1</sup> , Michel Nieuwoudt <sup>1</sup> , <u>Claude Agueraray</u> <sup>1</sup> <sup>1</sup> The University of Auckland <sup>2</sup> Counties Manukau District Health Board <sup>3</sup> Department of Dermatology, Middlemore Hospital <sup>4</sup> Department of Plastic Surgery, Middlemore Hospital
11:05-11:20		<b>Self-assembled nanogap arrays of gold nanoparticles in dimple nanopores induced by DNA hybridization</b> Hajun Dang <sup>1</sup> , Jaebum Choo <sup>1</sup> <sup>1</sup> Chung-Ang University
11:25-11:35		<b>An injectable biosensor for continuous remote monitoring of patients with prostate cancer</b> <u>Marta Aranda Palomer</u> <sup>1</sup> , Maria S. Relvas <sup>2</sup> , Sergio Quintero <sup>1</sup> , Jason B. King <sup>3</sup> , Mengkun Chen <sup>3</sup> , James W. Tunnell <sup>3</sup> , Ana Oliveira <sup>4</sup> , Pedro Costa <sup>5</sup> , Rui Sousa <sup>5</sup> , Adriana Mendes <sup>6</sup> , Olga Martinho <sup>6</sup> , Fatima Baltazar <sup>6</sup> , Lorena Dieguez <sup>1</sup> , Sara Abalde-Cela <sup>1</sup> <sup>1</sup> International Iberian Nanotechnology Laboratory (INL) <sup>2</sup> International Iberian Nanotechnology laboratory (INL) <sup>3</sup> University of Texas at Austin (UTA) <sup>4</sup> Stemmaters Biotecnologia e Medicina Regenerativa SA <sup>5</sup> Stemmaters Biotecnologia e Medicina Regenerativa <sup>6</sup> Life and Health Research Institute (ICVS)

11:40-11:50		<b>Dual nano-heater and SERS temperature sensor for cancer photothermal therapy</b> William H. Skinner <sup>1</sup> , Renata L. Sala <sup>2</sup> , Kamil Sokolowski <sup>2</sup> , Jeremy J. Baumberg <sup>2</sup> , Oren A. Scherman <sup>2</sup> , Benjamin Gardner <sup>1</sup> , Pavel Matousek <sup>3</sup> , Nicholas Stone <sup>1</sup> <sup>1</sup> University of Exeter <sup>2</sup> University of Cambridge <sup>3</sup> STFC Rutherford Appleton Laboratory
11:55-12:05		<b>Blood pulse dynamics investigation with non-invasive Raman spectroscopy</b> Maciej Wróbel <sup>1</sup> <sup>1</sup> Gdansk University of Technology
12:10-13:10		<b>Lunch</b>
13:10-14:30		<b>SESSION 2</b>
	A1-01	<b>(I) Chemometrics&amp;machine learning</b> Chair: Katarzyna Cieřlik-Boczula
13:10-13:25		<b>Two-trace two-dimensional (2T2D) FTIR correlation spectra applied as input</b> Bogumiła Kupcewicz <sup>1</sup> <sup>1</sup> Nicolaus Copernicus University, Faculty of Pharmacy
13:30-13:40		<b>Decoupling of morphological and chemical information in <math>\mu</math>FTIR spectra using deep learning</b> Uladzislau Blazhko <sup>1</sup> , Eirik Magnussen <sup>1</sup> , Johanne Solheim <sup>1</sup> , Simona Dzurendova <sup>1</sup> , Volha Shapaval <sup>1</sup> , Achim Kohler <sup>1</sup> <sup>1</sup> Norwegian University of Life Sciences
13:45-13:55		<b>Investigation of the bread aging process by handheld NIR spectroscopy in tandem with 2D-COS and MCR-ALS analyses</b> Marina De Géa Neves <sup>1</sup> , Isao Noda <sup>2</sup> , Heinz Wilhelm Siesler <sup>1</sup> <sup>1</sup> Department of Physical Chemistry, University Duisburg-Essen <sup>2</sup> Department of Materials Science and Engineering, University of Delaware
14:00-14:10		<b>Can we follow the metabolism of single leukemic cells using Raman spectroscopy?</b> Anna M. Nowakowska <sup>1</sup> , Aleksandra Borek-Doros <sup>1</sup> , Patrycja Dawiec <sup>2</sup> , Patrycja Leszczenko <sup>2</sup> , Adriana Adamczyk <sup>2</sup> , Kacper Siakala <sup>1</sup> , Justyna Jakubowska <sup>3</sup> , Marta Zabczynska <sup>3</sup> , Agata Pastorczak <sup>3</sup> , Kinga Ostrowska <sup>3</sup> , Wojciech Mlynarski <sup>3</sup> , Małgorzata Baranska <sup>4</sup> , Katarzyna Majzner <sup>1</sup> <sup>1</sup> Jagiellonian University in Krakow, Faculty of Chemistry, Department of Chemical Physics, Krakow, Poland <sup>2</sup> Jagiellonian University in Krakow, Faculty of Chemistry, Department of Chemical Physics, Krakow, Poland; Doctoral School of Exact and Natural Sciences, Jagiellonian University, Krakow, Poland <sup>3</sup> Department of Pediatric, Oncology and Hematology, Medical University of Lodz, Lodz, Poland <sup>4</sup> Jagiellonian University in Krakow, Faculty of Chemistry, Department of Chemical Physics, Krakow, Poland; Jagiellonian University in Krakow, Jagiellonian Centre for Experimental Therapeutics (JCET), Krakow, Poland
	A1-02	<b>(E) Nonlinear vibrational spectroscopy</b> Chair: Xiang Wang
13:10-13:25		<b>Specific Ion Effects in the Electrical Double Layer Structure at the Silica/Aqueous Interface</b> Julianne Gibbs <sup>1</sup> , Nathaniel Tetteh <sup>1</sup> , Shyam Parshotam <sup>1</sup> <sup>1</sup> University of Alberta
13:30-13:45		<b>Mechanistic Approach to Investigate the Water Evaporation Process at Air/Water Interface using Hofmeister Ions</b> Bhawna Rana <sup>1</sup> , David J. Fairhurst <sup>2</sup> , Kailash C. Jena <sup>1</sup> <sup>1</sup> Indian Institute of Technology Ropar <sup>2</sup> Nottingham Trent University
13:50-14:00		<b>Ultrafast decay of coupled molecule-plasmon nanogap structure</b> Fiona Bell <sup>1</sup> , Lukas Jakob <sup>1</sup> , Ishaan Lohia <sup>1</sup> , Rakesh Arul <sup>1</sup> , Jeremy Baumberg <sup>1</sup> <sup>1</sup> University of Cambridge
14:05-14:15		<b>How and when does the collapse of a macromolecule in water start? From time-resolved Raman to elastic light scattering viewpoint.</b> Marcin Pastorczak <sup>1</sup> , Michał Nejbauer <sup>1</sup> , Naoki Shinyashiki <sup>2</sup> , Masanobu Takatsuka <sup>2</sup> , Gonzalo Angulo <sup>1</sup> , Yuriy Stepanenko <sup>1</sup> , Czesław Radzewicz <sup>3</sup> <sup>1</sup> Institute of Physical Chemistry Polish Academy of Sciences <sup>2</sup> Department of Physics, School of Science, Tokai University <sup>3</sup> Institute of Experimental Physics, Faculty of Physics, University of Warsaw

14:20-14:30		<b>Taking Advantage of High Sensitivity Enabled by Stimulated Raman Scattering: Multi-Parameter Analysis of Nanoplastics in Flow</b> Maximilian Huber <sup>1</sup> , Liron Zada <sup>2</sup> , Freek Arieze <sup>2</sup> , Natalia P. Ivleva <sup>1</sup> <sup>1</sup> Technical University of Munich, Institute of Water Chemistry, Chair of Analytical Chemistry and Water Chemistry, School of Natural Sciences (Dep. Chemistry) <sup>2</sup> Vrije Universiteit Amsterdam, LaserLaB Amsterdam, Department of Physics and Astronomy
	A0-04	<b>(F) Advances in instrumentation</b> Chair: Yuling Wang
13:10-13:20		<b>Mid-IR Dispersion Spectroscopy – A Powerful Tool for Liquid-Phase Chemical Analysis</b> Alicja Dabrowska <sup>1</sup> , Bernhard Lendl <sup>1</sup> <sup>1</sup> Technische Universität Wien
13:25-13:35		<b>Raman spectrometer with vertical flow method for organic solvents</b> Ting-hao Chen <sup>1</sup> , Hirotsugu Hiramatsu <sup>1</sup> <sup>1</sup> Department of Applied Chemistry and Institute of Molecular Science, National Yang Ming Chiao Tung University
13:40-13:50		<b>High-performance miniaturized Raman systems for challenging Raman spectroscopy and microscopy applications</b> Oleksii Ilchenko <sup>1</sup> , Yurii Pilhun <sup>2</sup> , Andrii Kutsyk <sup>1</sup> , Yaman Goksel <sup>1</sup> , Elodie Dumont <sup>1</sup> , Thomas Andersen <sup>3</sup> , Mikael Lassen <sup>4</sup> , Hemanshu Mundhada <sup>5</sup> , Christian Jendresen <sup>5</sup> , Anja Boisen <sup>1</sup> <sup>1</sup> Technical University of Denmark <sup>2</sup> Lightnovo ApS <sup>3</sup> Odense University Hospital <sup>4</sup> Danish National Metrology Institute <sup>5</sup> Cysbio ApS
13:55-14:05		<b>A correlated OF2i®-Raman method for micro- and nanoparticle detection and chemical analysis in liquids</b> Christian Neuper <sup>1</sup> , Marko Šimić <sup>2</sup> , Christian Hill <sup>3</sup> , Werner Grogger <sup>4</sup> , Harald Fitzek <sup>5</sup> <sup>1</sup> Graz Centre of Electron Microscopy, Steyrergasse 17, Austria / Brave Analytics GmbH, Austria <sup>2</sup> Brave Analytics GmbH, Austria / Gottfried Schatz Research Center, Division of Biophysics, Medical University of Graz, Neue Stiftingtalstraße 2, Graz 8010, Austria / Institute of Physics, University of Graz, Universitätsplatz 5, Graz 8010, Austria <sup>3</sup> Brave Analytics GmbH, Austria / Gottfried Schatz Research Center, Division of Biophysics, Medical University of Graz, Neue Stiftingtalstraße 2, Graz 8010, Austria <sup>4</sup> Graz Centre of Electron Microscopy, Steyrergasse 17, Austria / Institute of Electron Microscopy and Nanoanalysis, NAWI Graz, Graz University of Technology, Steyrergasse 17, Austria <sup>5</sup> Graz Centre of Electron Microscopy, Steyrergasse 17, Austria
14:10-14:20		<b>Dielectrophoresis for Raman analysis in liquid: towards a rapid and label-free platform for virus identification</b> Alessio Sacco <sup>1</sup> , Giulia Barzan <sup>1</sup> , Slavica Matić <sup>2</sup> , Chiara D'Errico <sup>2</sup> , Marta Vallino <sup>2</sup> , Marina Ciuffo <sup>2</sup> , Emanuela Noris <sup>2</sup> , Andrea Mario Giovannozzi <sup>1</sup> , Chiara Portesi <sup>1</sup> , Andrea Mario Rossi <sup>1</sup> <sup>1</sup> National Metrology Research Institute (INRiM) <sup>2</sup> Institute for Sustainable Plant Protection, National Research Council of Italy (CNR)
14:25-14:35		<b>A Tailored Setup for Multiphase In situ Spectroscopy on Gas-processing Metalloenzymes</b> Christian Lorent <sup>1</sup> , Sagie Katz <sup>1</sup> , Vladimir Pelmenschikov <sup>1</sup> , Giorgio Caserta <sup>1</sup> , Stefan Frielingsdorf <sup>1</sup> , Maria Alessandra Martini <sup>2</sup> , Konstantin Bikbaev <sup>3</sup> , Ingrid Span <sup>3</sup> , James A.F. Birrell <sup>4</sup> , Oliver Lenz <sup>1</sup> , Marius Horch <sup>5</sup> , Ingo Zebger <sup>1</sup> <sup>1</sup> Technische Universität Berlin, Institut für Chemie <sup>2</sup> Max-Planck-Institut für Chemische Energiekonversion <sup>3</sup> Friedrich-Alexander-Universität Erlangen-Nürnberg <sup>4</sup> University of Essex, School of Life Sciences <sup>5</sup> Freie Universität Berlin, Institut für Physik, Biophysik
	A0-03	<b>(G) Analytical applications</b> Chair: Natalia Ivleva
13:10-13:20		<b>Novel Analytical Approach for Rapid Detection and Characterization of Microplastics in Environmental Samples: Utilizing MIR Spectroscopy's Silent Region for Enhanced Structural Information</b> Krzysztof B. Bec <sup>1</sup> , Justyna Grabska <sup>1</sup> , Jovan Badzoka <sup>1</sup> , Christian W. Huck <sup>1</sup> <sup>1</sup> University of Innsbruck

13:25-13:35		<b>Quantification of microplastics in environmental samples through a combination of optical and FTIR- and Raman microspectroscopy enhanced by Machine Learning evaluation</b> Dieter Fischer <sup>1</sup> , Kristina Enders <sup>1</sup> , Robin Lenz <sup>1</sup> , Franziska Fischer <sup>2</sup> , Elisavet Kanaki <sup>1</sup> , Julia Muche <sup>1</sup> , Benedikt Hufnagel <sup>3</sup> <sup>1</sup> Leibniz-Institut für Polymerforschung Dresden <sup>2</sup> Advanced Mask Technology Center GmbH Dresden <sup>3</sup> Purency GmbH Wien
13:40-13:50		<b>Comparison of Raman- and fluorescence techniques for detection and identification of microplastics in environmental samples</b> Merel Konings <sup>1</sup> , Liron Zada <sup>1</sup> , Robert Schmidt <sup>1</sup> , Freek Arie <sup>1</sup> <sup>1</sup> Vrije Universiteit Amsterdam
13:55-14:05		<b>Applications of optical photothermal infrared spectroscopy (O-PTIR) in plastic pollution research: from detecting microplastics to monitoring the production of microbial bioplastic</b> Cassio Lima <sup>1</sup> , Howbeer Muhamadali <sup>1</sup> , Royston Goodacre <sup>1</sup> <sup>1</sup> University of Liverpool
14:10-14:20		<b>Nanoscale chemical characterization is crucial for polymer recycling</b> Georg Ramer <sup>1</sup> , V. D. Dos Santos A. Catarina <sup>1</sup> , Lena Neubauer <sup>2</sup> , Bernhard Lendl <sup>2</sup> <sup>1</sup> TU Wien / Institute for chemical Technologies and Analytics <sup>2</sup> TU Wien / Institute for chemical Technologie and Analytics
14:25-14:35		<b>In-line near-infrared spectroscopic monitoring for injection molding of biodegradable polymer blends</b> Itsuki Yoshikawa <sup>1</sup> , Yuta Hikima <sup>1</sup> , Masahiro Ohshima <sup>1</sup> <sup>1</sup> Kyoto University
	A0-01	<b>(H) Biodiagnostic spectroscopy</b> Chair: Peter Gardner
13:10-13:20		<b>Rapid identification of bacteria isolated directly from patient urine and diagnosis of their antibiotic susceptibility using infrared spectroscopy-based machine learning</b> George Abu-Aqil <sup>1</sup> , Manal Suleiman <sup>1</sup> , Uraib Sharaha <sup>1</sup> , Lior Nesher <sup>2</sup> , Itshak Lapidot <sup>3</sup> , Ahmad Salman <sup>4</sup> , Mahmoud Huleihel <sup>1</sup> <sup>1</sup> Ben-Gurion University of the Negev <sup>2</sup> Soroka University Medical Center <sup>3</sup> Afeka Tel-Aviv Academic College of Engineering <sup>4</sup> Shamoon College of Engineering
13:25-13:35		<b>Supplementation of vitamin C and E – an effect on human gastrointestinal tract tissues and cells: Raman spectroscopy and imaging</b> Karolina Beton-Mysur <sup>1</sup> , Beata Brożek-Płuska <sup>1</sup> <sup>1</sup> Lodz University of Technology, Faculty of Chemistry, Institute of Applied Radiation Chemistry, Laboratory of Laser Molecular Spectroscopy
13:40-13:50		<b>Molecular Characterisation of T-cell acute lymphoblastic leukemia using Raman spectroscopy</b> Patrycja Dawiec <sup>1</sup> , Patrycja Leszczenko <sup>1</sup> , Anna Nowakowska <sup>2</sup> , Karolina Czuja <sup>2</sup> , Justyna Jakubowska <sup>3</sup> , Marta Zabczyńska <sup>3</sup> , Agata Pastorczak <sup>3</sup> , Kinga Ostrowska <sup>3</sup> , Wojciech Mlynarski <sup>3</sup> , Malgorzata Baranska <sup>4</sup> , Katarzyna Majzner <sup>2</sup> <sup>1</sup> Jagiellonian University in Krakow, Faculty of Chemistry, Department of Chemical Physics; Doctoral School of Exact and Natural Sciences <sup>2</sup> Jagiellonian University in Krakow, Faculty of Chemistry, Department of Chemical Physics <sup>3</sup> Department of Pediatrics, Oncology and Hematology, Medical University of Lodz <sup>4</sup> Jagiellonian University in Krakow, Faculty of Chemistry, Department of Chemical Physics; Jagiellonian University in Krakow, Jagiellonian Centre for Experimental Therapeutics
13:55-14:05		<b>Raman-based assessment of the endothelial response to antiretroviral drugs: in vitro studies on NNRTI-treated human endothelial cells</b> Jagoda Orleanska <sup>1</sup> , Wiktoria Wiecek <sup>2</sup> , Malgorzata Baranska <sup>3</sup> , Katarzyna Majzner <sup>2</sup> <sup>1</sup> 1 Jagiellonian University, Faculty of Chemistry, Department of Chemical Physics, Krakow, Poland; 2 Doctoral School of Exact and Natural Sciences, Jagiellonian University in Krakow, Krakow, Poland <sup>2</sup> 1 Jagiellonian University, Faculty of Chemistry, Department of Chemical Physics, Krakow, Poland <sup>3</sup> 1 Jagiellonian University, Faculty of Chemistry, Department of Chemical Physics, Krakow, Poland; 3 Jagiellonian University in Krakow, Jagiellonian Centre for Experimental Therapeutics (JCET), Krakow, Poland

14:10-14:20		<b>Bladder Cancer detection by Fourier Transform Infrared Spectroscopy (FTIR) using urine samples.</b> Imane Oudahmane <sup>1</sup> , Fayek Taha <sup>2</sup> , Elie Sarkees <sup>1</sup> , Jade Vanmansart <sup>1</sup> , Vincent Vuiblet <sup>3</sup> , Stéphane Larre <sup>2</sup> , Olivier Piot <sup>1</sup> <sup>1</sup> BioSpect (Translational BioSpectroscopy) EA 7506. Université de Reims Champagne-Ardenne. <sup>2</sup> Department of Urology, University Hospital of Reims. <sup>3</sup> Department of Biopathology, University Hospital of Reims.
14:25-14:35		<b>Exploring the potential for Deep Raman Spectroscopy for non-invasive sex determination of chicken eggs</b> Lennard Van den Tweel <sup>1</sup> , Freek Arieze <sup>2</sup> , Carla Van der Pol <sup>3</sup> , Henry Van den Brand <sup>1</sup> <sup>1</sup> Adaptation Physiology Group, Wageningen University & Research <sup>2</sup> LaserLaB, Department of Physics and Astronomy, Vrije Universiteit Amsterdam <sup>3</sup> Research Department, HatchTech B.V.
14:30-15:00		<b>Coffee Break</b>
15:00-16:15		<b>SESSION 3</b>
	A1-01	<b>(I) Chemometrics&amp;machine learning</b> Chair: Stefania Dana Iancu
15:00-15:10		<b>Advancing cancer stem cell detection through line illumination Raman microscope and hydrogel substrate.</b> Jean-Emmanuel Clément <sup>1</sup> , Zannatul Ferdous <sup>1</sup> , Thomas Bocklitz <sup>2</sup> , Katsumasa Fujita <sup>3</sup> , Jian Ping Gong <sup>1</sup> , Shinya Tanaka <sup>1</sup> , Tamiki Komatsuzaki <sup>1</sup> <sup>1</sup> Hokkaido University-ICReDD <sup>2</sup> University of Bayreuth <sup>3</sup> Osaka University
15:15-15:25		<b>Discrimination between chemoresistant and chemosensitive ovarian cancer cells with confocal Raman microscopy</b> Elina Harju <sup>1</sup> , Teemu Tomberg <sup>1</sup> , Sara Fraser-Miller <sup>2</sup> , Jukka Saarinen <sup>1</sup> , Kathleen J. Sircombe <sup>3</sup> , Sarah Hook <sup>3</sup> , Keith C. Gordon <sup>2</sup> , Clare J. Strachan <sup>1</sup> <sup>1</sup> Division of Pharmaceutical Chemistry and Technology, Faculty of Pharmacy, University of Helsinki <sup>2</sup> The Dodd-Walls Centre for Photonic and Quantum Technologies – Te Whai Ao and Department of Chemistry, University of Otago <sup>3</sup> School of Pharmacy, University of Otago
15:30-15:40		<b>Can we diagnose the KMT2A leukemia subtype with Raman microscopy?</b> Patrycja Leszczenko <sup>1</sup> , Anna M. Nowakowska <sup>1</sup> , Justyna Jakubowska <sup>2</sup> , Agata Pastorczak <sup>2</sup> , Marta Zabczynska <sup>2</sup> , Wojciech Mlynarski <sup>2</sup> , Malgorzata Baranska <sup>1</sup> , Kinga Ostrowska <sup>2</sup> , Katarzyna Majzner <sup>1</sup> <sup>1</sup> Faculty of Chemistry, Jagiellonian University <sup>2</sup> Department of Pediatric, Oncology and Hematology, Medical University of Lodz
15:45-15:55		<b>Pretreatment routines in analysis of Raman spectra recorded in different excitation wavelength and its effect on classification models</b> Sara Mostafapour <sup>1</sup> , Thomas Dörfer <sup>2</sup> , Ralf Henke <sup>2</sup> , Petra Röscher <sup>2</sup> , Jürgen Popp <sup>1</sup> , Thomas Bocklitz <sup>3</sup> <sup>1</sup> 1. Leibniz Institute of Photonic Technology, Jena, Germany/2. Institute of Physical Chemistry and Abbe Centre of Photonics, Friedrich Schiller University of Jena, Jena, Germany <sup>2</sup> Institute of Physical Chemistry and Abbe Centre of Photonics, Friedrich Schiller University of Jena, Jena, Germany <sup>3</sup> 1. Leibniz Institute of Photonic Technology, Jena, Germany/2. Institute of Physical Chemistry and Abbe Centre of Photonics, Friedrich Schiller University of Jena, Jena, Germany/3. Institute of Computer Science, Faculty of Mathematics, Physics & Computer Sc
16:00-16:10		<b>Infrared molecular fingerprinting for multi-phenotyping of human health and disease</b> Kepesidis V. Kosmas <sup>1</sup> , Marinus Huber <sup>2</sup> , Liudmila Voronina <sup>1</sup> , Tarek Eissa <sup>1</sup> , Frank Fleischmann <sup>1</sup> , Cristina Leonardo <sup>1</sup> , Jacqueline Hermann <sup>1</sup> , Ina Koch <sup>3</sup> , Thomas Kolben <sup>4</sup> , Gerald Schulz <sup>5</sup> , Friedrich Jokisch <sup>5</sup> , Juergen Behr <sup>6</sup> , Nadia Harbeck <sup>4</sup> , Maximilian Reiser <sup>7</sup> , Christian Stief <sup>5</sup> , Ferenc Krausz <sup>1</sup> , Mihaela Zigman <sup>1</sup> <sup>1</sup> Ludwig Maximilian University of Munich (LMU) <sup>2</sup> Max Planck Institute of Quantum Optics (MPQ) <sup>3</sup> Asklepios Biobank for Lung Diseases, Department of Thoracic Surgery, Member of the German Center for Lung Research, DZL, Asklepios Fachkliniken München-Gauting <sup>4</sup> University Hospital of the Ludwig Maximilians University Munich (LMU), Department of Obstetrics and Gynecology, Breast Center and Comprehensive Cancer Center (CCLMU) <sup>5</sup> University Hospital of the Ludwig Maximilians University Munich (LMU), Department of Urology <sup>6</sup> University Hospital of the Ludwig Maximilians University Munich (LMU), Department of Internal Medicine V <sup>7</sup> University Hospital of the Ludwig Maximilians University Munich (LMU), Department of Clinical Radiology



	A1-02	<b>(E) Nonlinear vibrational spectroscopy</b> Chair: Marcin Pastorczak
15:00-15:10		<b>Raman and Stimulated Raman Scattering characterization of carotenoids and amyloid beta deposits in Alzheimer's Disease brain samples</b> Freek Arie <sup>1</sup> , Benjamin Lochocki <sup>2</sup> , Liron Zada <sup>1</sup> , Loes Ettema <sup>1</sup> , Can Keskin <sup>1</sup> , Jinke Van der Sluis <sup>1</sup> , Robert W. Schmidt <sup>1</sup> <sup>1</sup> LaserLaB, Vrije Universiteit <sup>2</sup> ARCNL
15:15-15:25		<b>Glucose and lipid metabolism in endothelium inflammation studied by Raman microscopy</b> Aleksandra Borek-Dorosz <sup>1</sup> , Anna Pieczara <sup>2</sup> , Jagoda Orleańska <sup>3</sup> , Krzysztof Brzozowski <sup>1</sup> , William Tipping <sup>4</sup> , Duncan Graham <sup>4</sup> , Małgorzata Barańska <sup>5</sup> , Katarzyna Majzner <sup>1</sup> <sup>1</sup> Jagiellonian University in Kraków, Faculty of Chemistry, Department of Chemical Physics, 2 Gronostajowa Str., Krakow, Poland <sup>2</sup> Jagiellonian University in Kraków, Jagiellonian Centre for Experimental Therapeutics (JCET), 14 Bobrzynskiego Str., Krakow, Poland <sup>3</sup> Jagiellonian University in Kraków, Doctoral School of Exact and Natural Sciences, 11 Łojasiewicza St., Krakow, Poland <sup>4</sup> Jagiellonian University in Kraków, Faculty of Chemistry, Department of Chemical Physics, 2 Gronostajowa Str., Krakow, Poland <sup>5</sup> Jagiellonian University in Kraków, Doctoral School of Exact and Natural Sciences, 11 Łojasiewicza St., Krakow, Poland <sup>4</sup> Centre for Molecular Nanometrology, WestCHEM, Department of Pure and Applied Chemistry, Technology and Innovation Centre, University of Strathclyde, Glasgow G1 1RD, United Kingdom <sup>5</sup> Jagiellonian University in Kraków, Faculty of Chemistry, Department of Chemical Physics, 2 Gronostajowa Str., Krakow, Poland <sup>2</sup> Jagiellonian University in Kraków, Jagiellonian Centre for Experimental Therapeutics (JCET), 14 Bobrzynskiego Str., Krakow, Poland
15:30-15:40		<b>Stimulated Raman scattering imaging – 3D spatial generation</b> Ronja Eriksson <sup>1</sup> , Per Gren <sup>1</sup> , Mikael Sjö Dahl <sup>1</sup> , Kerstin Ramser <sup>1</sup> <sup>1</sup> Department of Engineering Sciences and Mathematics, Luleå University of Technology
15:45-15:55		<b>Modified glucose as a probe to track the metabolism in single endothelial cells – observation of the 1602 cm<sup>-1</sup> band called “Raman spectroscopic signature of life”</b> Anna Pieczara <sup>1</sup> , Aleksandra Borek-Dorosz <sup>1</sup> , Szymon Buda <sup>1</sup> , William Tipping <sup>2</sup> , Duncan Graham <sup>2</sup> , Robert Pawłowski <sup>3</sup> , Jacek Młynarski <sup>3</sup> , Małgorzata Barańska <sup>1</sup> <sup>1</sup> Jagiellonian University <sup>2</sup> University of Strathclyde <sup>3</sup> Polish Academy of Sciences
16:00-16:10		<b>Stimulated Raman scattering (SRS) microscopy to investigate pharmaceutical co-crystal formation</b> Oona Auvinen <sup>1</sup> , Alba Arbiol <sup>1</sup> , Tom Konings <sup>1</sup> , Teemu Tomberg <sup>1</sup> , Leena Peltonen <sup>1</sup> , Clare Strachan <sup>1</sup> , Jukka Saarinen <sup>1</sup> <sup>1</sup> Division of Pharmaceutical Chemistry and Technology, Faculty of Pharmacy, University of Helsinki
	A0-04	<b>(A) Advanced characterization of materials</b> Chair: Justyna Grabska
15:00-15:15		<b>Inside block copolymer micelles – An AFM-TERS study on the interfacial influences on the core crosslinking efficiency</b> Christiane Höppener <sup>1</sup> , Xinyue Wang <sup>2</sup> , Johanna Elter <sup>3</sup> , Felix Schacher <sup>3</sup> , Volker Deckert <sup>1</sup> <sup>1</sup> Leibniz Institute of Photonic Technologies (IPHT) <sup>2</sup> Institute of Physical Chemistry, Friedrich Schiller University <sup>3</sup> Institute of Organic Chemistry and Macromolecular Chemistry, Friedrich Schiller University
15:20-15:35		<b>Towards the compactness and permeability of the polymer brushes studied by surface-enhanced Raman spectroscopy</b> Marek Procházka <sup>1</sup> , Monika Spasovová <sup>2</sup> , Markéta Vrabcová <sup>2</sup> , Josef Štěpánek <sup>1</sup> , Ondřej Kylián <sup>3</sup> , Hana Vaisocherová-Lísalová <sup>4</sup> <sup>1</sup> Institute of Physics, Faculty of Mathematics and Physics, Charles University <sup>2</sup> Department of Optical and Biophysical Systems, Institute of Physics of the Czech Academy of Sciences; Institute of Physics, Faculty of Mathematics and Physics, Charles University <sup>3</sup> Department of Macromolecular Physics, Faculty of Mathematics and Physics, Charles University <sup>4</sup> Department of Optical and Biophysical Systems, Institute of Physics of the Czech Academy of Sciences

15:40-15:50		<b>Characterisation and evaluation of molecularly imprinted polymers using surface enhanced infrared absorption (SEIRA) spectroscopy.</b> Armel F. T. Waffo <sup>1</sup> , Sagie Katz <sup>1</sup> , Giorgio Caserta <sup>1</sup> , Aysu Yarman <sup>2</sup> , Bettina Neumann <sup>3</sup> , Ulla Wollenberger <sup>3</sup> , Frieder W. Scheller <sup>3</sup> <sup>1</sup> Technische Universität Berlin <sup>2</sup> Turkish-German University <sup>3</sup> University of Potsdam
15:55-16:05		<b>Enhancement of the E12g and A1g Raman modes and Layer Identification of 2H-WS2 Nanosheets With Metal Coatings</b> Bharathi Rajeswaran <sup>1</sup> , Rajashree Konar <sup>1</sup> , Gilbert Daniel Nessim <sup>2</sup> , Yaakov Raphael Tischler <sup>1</sup> <sup>1</sup> Bar-Ilan University, Israel <sup>2</sup> Bar-Ilan University, Ramat Gan, Israel
	A0-03	<b>(G) Analytical applications</b> Chair: Maria-Paula Marques
15:00-15:15		<b>Insights into forensic analysis of peripheral blood stains on natural and synthetic fabrics using ATR-FTIR spectroscopy</b> Entesar Al-Hetlani <sup>1</sup> , Zainab Husain <sup>1</sup> , Mohamed Amin <sup>1</sup> <sup>1</sup> Kuwait University
15:20-15:35		<b>Revealing the Secrets of Graeco-Roman Egyptian Mummies Using Vibrational Spectroscopic Techniques</b> Bayden Wood <sup>1</sup> , Callum Gassner <sup>1</sup> , Magdalena Giergiel <sup>1</sup> , Ankit Dodla <sup>1</sup> , Janet Davey <sup>2</sup> <sup>1</sup> Monash University <sup>2</sup> Victorian Institute of Forensic Medicine
15:40-15:50		<b>Fingermark analysis utilizing ATR-FTIR spectroscopy for forensic discrimination of smoker and nonsmoker</b> Mohamed O. Amin <sup>1</sup> , Entesar Al-Hetlani <sup>1</sup> , Igor K. Lednev <sup>2</sup> <sup>1</sup> Kuwait University <sup>2</sup> University at Albany
15:55-16:05		<b>Deep UV Raman spectroscopy for post-mortem interval determination</b> Anna Wójtowicz <sup>1</sup> , Luis Perez Almodovar <sup>2</sup> , Igor K. Lednev <sup>2</sup> , Renata Wietecha-Postuszny <sup>1</sup> <sup>1</sup> Laboratory for Forensic Chemistry, Department of Analytical Chemistry, Faculty of Chemistry, Jagiellonian University <sup>2</sup> Department of Chemistry, University at Albany, SUNY
	A0-01	<b>(H) Biodiagnostic spectroscopy</b> Chair: Hugh Byrne
15:00-15:10		<b>Raman-based evaluation of in vitro myeloid precursor differentiation toward macrophages</b> Adriana Adamczyk <sup>1</sup> , Anna Nowakowska <sup>1</sup> , Justyna Jakubowska <sup>2</sup> , Katarzyna Majzner <sup>1</sup> , Malgorzata Baranska <sup>1</sup> <sup>1</sup> Jagiellonian University in Krakow, Faculty of Chemistry, Department of Chemical Physics, Kraków, Poland <sup>2</sup> Department of Pediatrics, Oncology and Hematology, Medical University of Lodz, Łódź, Poland
15:15-15:25		<b>Brillouin and Raman micro-spectroscopy to characterise human bone and cartilage: from healthy phenotype to biomedical applications in osteoarthritis and bone infections.</b> Martina Alunni Cardinali <sup>1</sup> , Sara Stefani <sup>1</sup> , Marco Govoni <sup>2</sup> , Dante Dallari <sup>2</sup> , Leonardo Vivarelli <sup>2</sup> , Matilde Tschon <sup>3</sup> , Silvia Brogini <sup>3</sup> , Alessandra Maso <sup>4</sup> , Elisa Storni <sup>4</sup> , Francesca Valenti <sup>5</sup> , Melania Maglio <sup>3</sup> , Maurizio Mattarelli <sup>6</sup> , Alessandra Anna Passeri <sup>6</sup> , Silvia Caponi <sup>7</sup> , Assunta Morresi <sup>1</sup> , Paola Sassi <sup>1</sup> , Daniele Fioretto <sup>6</sup> <sup>1</sup> Dep. Chemistry, Biology and Biotechnology, University of Perugia <sup>2</sup> Reconstructive Orthopaedic Surgery and Innovative Techniques – Musculoskeletal Tissue Bank, IRCCS Istituto Ortopedico Rizzoli <sup>3</sup> Surgical Sciences and Technologies, IRCCS Istituto Ortopedico Rizzoli <sup>4</sup> Laboratory of Microbiology and GMP Quality Control, IRCCS Istituto Ortopedico Rizzoli <sup>5</sup> Dep. of Pharmacy and Biotechnology, University of Bologna <sup>6</sup> Dep. Physics and Geology, University of Perugia <sup>7</sup> CNR- Dep. Physics and Geology

15:30-15:40		<b>Fourier Transform Infrared Microspectroscopy identifies single cancer cells in blood. A feasibility study towards liquid biopsy.</b> Lewis M. Dowling <sup>1</sup> , Paul Roach <sup>2</sup> , Eirik A. Magnussen <sup>3</sup> , Achim Kohler <sup>3</sup> , Srinivas Pillai <sup>4</sup> , Daniel G. Van Pittius <sup>4</sup> , Ibraheem Yousef <sup>5</sup> , Josep Sulé-Suso <sup>1</sup> <sup>1</sup> Keele University <sup>2</sup> Loughborough University <sup>3</sup> Norwegian University of Life Sciences <sup>4</sup> University Hospitals of North Midlands <sup>5</sup> ALBA Synchrotron Light Source
15:45-15:55		<b>Raman spectroscopy in the biochemical characterisation of THP-1 leukemic cells modified to overexpress mutated FLT3 receptor.</b> Sylwia Orzechowska <sup>1</sup> , Paulina Laskowska <sup>2</sup> , Aleksandra Borek-Dorosz <sup>1</sup> , Anna Maria Nowakowska <sup>1</sup> , Wiktoria Korona <sup>1</sup> , Marcin Szydłowski <sup>2</sup> , M. Zasowska <sup>2</sup> , Piotr Juszczynski <sup>2</sup> , Małgorzata Barańska <sup>3</sup> , Piotr Mrówka <sup>4</sup> , Katarzyna Majzner <sup>1</sup> <sup>1</sup> Jagiellonian University, Faculty of Chemistry <sup>2</sup> Department of Experimental Hematology, Institute of Hematology and Transfusion Medicine <sup>3</sup> Jagiellonian University, Faculty of Chemistry; Jagiellonian Centre for Experimental Therapeutics (JCET), Jagiellonian University <sup>4</sup> Department of Experimental Hematology, Institute of Hematology and Transfusion Medicine; Department of Biophysics, Physiology and Pathophysiology, Medical University of Warsaw
16:00-16:10		<b>Identification of Chemical Modifications of Myocardium in Heart-Failure with Preserved Ejection Fraction</b> Leonardo Pioppi <sup>1</sup> , Reza Parvan <sup>2</sup> , Alan Samrend <sup>2</sup> , Gustavo Jose Justo Da Silva <sup>2</sup> , Marco Paolantoni <sup>1</sup> , Alessandro Cataliotti <sup>2</sup> , Paola Sassi <sup>1</sup> <sup>1</sup> Department of Chemistry, Biology and Biotechnology, University of Perugia <sup>2</sup> Institute for Experimental Medical Research, Oslo University Hospital and University of Oslo
16:30-18:45		<b>POSTER SESSION 3: Topics G, H, I</b>
		Chairs: Sara Miller, Christian Johannessen
16:30-17:30	A0-01	Flash Presentations
17:30-18:45		Poster Session
<b>Thursday</b>		
9:00-10:15	A0-01	<b>Plenary Session</b>
		Chair: Pavel Matousek
9:00-9:30		Raman Imaging of Plant Cells: probing distribution and orientation of molecules Notburga Gierlinger <sup>1</sup> <sup>1</sup> University of Natural Resources and Life Sciences Vienna (BOKU)
		Chair: Petra Hellwig
9:40-10:10		<b>Theory is dead, long live theory: Hypothesis-centric machine learning in vibrational spectroscopy</b> Axel Mosig <sup>1</sup> <sup>1</sup> Ruhr University Bochum, Center for Protein Diagnostics
10:15-10:45		<b>Coffee Break</b>
10:45-12:10		<b>SESSION 1</b>
	A1-01	<b>(I) Chemometrics&amp;machine learning</b> Chair: Alicja Dąbrowska
10:45-10:55		<b>Spatially offset low frequency Raman spectroscopy for discriminating microcalcifications immersed and under varying depths of paraffin wax</b> Mitchell Chalmers <sup>1</sup> , Sara Miller <sup>1</sup> , Teemu Tomberg <sup>2</sup> , Keith Gordon <sup>1</sup> <sup>1</sup> Te Whai Ao – The Dodd-Walls Centre for Photonic and Quantum Technologies and Department of Chemistry, University of Otago <sup>2</sup> Division of Pharmaceutical Chemistry and Technology, Faculty of Pharmacy, University of Helsinki
11:00-11:10		<b>The data exploring expedition. A practical outline to processing and investigation of experimental spectra with the selected methods of chemometric data modeling</b> Andrzej J. Kałka <sup>1</sup> , Andrzej M. Turek <sup>1</sup> <sup>1</sup> Jagiellonian University in Cracow, Faculty of Chemistry

11:15-11:25		<b>RamApp: a modern web-based toolbox for the processing and analysis of hyperspectral imaging data</b> Elia Broggio <sup>1</sup> , Andrea Masella <sup>1</sup> , Giulia De Poli <sup>1</sup> , Manuela Bazzarelli <sup>1</sup> , Dario Polli <sup>2</sup> , Matteo Bregonzio <sup>1</sup> , Renzo Vanna <sup>3</sup> <sup>1</sup> Datrix S.p.A. <sup>2</sup> Department of Physics, Politecnico di Milano / Istituto di Fotonica e Nanotecnologie (IFN), Consiglio Nazionale delle Ricerche (CNR) <sup>3</sup> Istituto di Fotonica e Nanotecnologie (IFN), Consiglio Nazionale delle Ricerche (CNR)
11:30-11:40		<b>Tensor decomposition assisted super-resolution in polarized Raman microscopy</b> Andrii Kutsyk <sup>1</sup> , Oleksii Ilchenko <sup>1</sup> , Yurii Pilhun <sup>2</sup> , Jens Wenzel Andreassen <sup>1</sup> <sup>1</sup> Technical University of Denmark <sup>2</sup> Lightnovo ApS
11:45-11:55		<b>Extensive Evaluation of Machine Learning Models and Data Preprocessings for Raman Modeling in Bioprocessing</b> Michaela Poth <sup>1</sup> , Gordon Magill <sup>2</sup> , Alois Filgertshofer <sup>1</sup> , Oliver Popp <sup>1</sup> , Tobias Großkopf <sup>1</sup> <sup>1</sup> Therapeutic Modalities, Roche Innovation Center Munich, Bioprocess Research, Roche Pharma Research and Early Development <sup>2</sup> Cell Culture Development and Bioprocess, Genentech Inc.
12:00-12:10		<b>Pre-Processing and Unsupervised Unmixing of Hyperspectral Raman Datasets with RamanLIGHT</b> Robert W. Schmidt <sup>1</sup> , Sander Woutersen <sup>2</sup> , Freek Arieze <sup>1</sup> <sup>1</sup> Vrije Universiteit Amsterdam <sup>2</sup> University of Amsterdam
	A1-02	<b>(E) Nonlinear vibrational spectroscopy</b> Chair: Zsuzsanna Heiner
10:45-11:00		<b>Nonlinear Vibrational Spectroscopy as an Orientation-Independent Probe of Molecular Environments at Interfaces</b> Dennis Hore <sup>1</sup> , Aruna Kumarasiri <sup>1</sup> , Peter Yang <sup>1</sup> <sup>1</sup> University of Victoria
11:05-11:20		<b>Molecular-Level Elucidation of Buried Solid/Liquid Interfaces by the Use of Heterodyne-detected Vibrational Sum Frequency Generation</b> Satoshi Nihonyanagi <sup>1</sup> <sup>1</sup> Molecular Spectroscopy Lab., RIKEN
11:25-11:35		<b>Investigating Viscoelastic Induced Nature at Air-Aqueous Interface by Nonlinear Laser Vibrational Spectroscopy</b> Sarabjeet Kaur <sup>1</sup> , Kailash Chandra Jena <sup>1</sup> <sup>1</sup> Indian Institute of Technology Ropar
11:40-11:50		<b>Unraveling the sign of excited-state molecular displacements via broadband impulsive Raman spectroscopy</b> Giovanni Batignani <sup>1</sup> , Emanuele Mai <sup>1</sup> , Giuseppe Fumero <sup>2</sup> , Shaul Mukamel <sup>3</sup> , Tullio Scopigno <sup>4</sup> <sup>1</sup> Physics Department, Sapienza University of Rome, Rome, Italy; Italian Institute of Technology, Center for Life Nano Science @Sapienza, Rome, Italy <sup>2</sup> Physics Department, Sapienza University of Rome, Rome, Italy <sup>3</sup> Department of Chemistry, University of California, Irvine, CA, USA <sup>4</sup> Physics Department, Sapienza University of Rome, Rome, Italy; Italian Institute of Technology, Center for Life Nano Science @Sapienza, Rome, Italy; Italian Institute of Technology, Graphene Labs, Genoa, Italy
11:55-12:05		<b>Charge Transfer Across Hydrophobic Interfaces</b> Saranya Pullanchery <sup>1</sup> , Sergey Kulik <sup>1</sup> , Benjamin Rehl <sup>1</sup> , Ali Hassanali <sup>2</sup> , Sylvie Roke <sup>1</sup> <sup>1</sup> Laboratory for Fundamental BioPhotonics, Institute of Bioengineering (IBI), School of Engineering (STI), École Polytechnique Fédérale de Lausanne (EPFL) <sup>2</sup> The Abdus Salam International Centre for Theoretical Physics

	A0-04	<b>(A) Advanced characterization of materials</b> Chair: Valentina Notarstefano
10:45-10:55		<b>Ibuprofen/chitosan matrices as a promising base for intestinal soft capsules</b> Barbara Gieroba <sup>1</sup> , Maryna Khalavka <sup>2</sup> , Olena Mozgova <sup>3</sup> , Paulina Kazmierczak <sup>4</sup> , Grzegorz Kalisz <sup>1</sup> , Izabela S. Pięta <sup>5</sup> , Liudmyla Nosach <sup>6</sup> , Vladyslav Vivcharenko <sup>4</sup> , Agata Przekora <sup>4</sup> , Anna Sroka-Bartnicka <sup>1</sup> <sup>1</sup> Independent Unit of Spectroscopy and Chemical Imaging, Faculty of Biomedical Sciences, Medical University of Lublin, Chodzki 4a, 20-093 Lublin, Poland <sup>2</sup> Independent Unit of Spectroscopy and Chemical Imaging, Faculty of Biomedical Sciences, Medical University of Lublin, Chodzki 4a, 20-093 Lublin, Poland; Department of Industrial Technology of Drugs, National University of Pharmacy, Pushkinska 63 St., 6100 <sup>3</sup> Independent Unit of Spectroscopy and Chemical Imaging, Faculty of Biomedical Sciences, Medical University of Lublin, Chodzki 4a, 20-093 Lublin, Poland; National University of Pharmacy, Department of Inorganic and Physical Chemistry, Valentynivska 4 St., 6 <sup>4</sup> Independent Unit of Tissue Engineering and Regenerative Medicine, Faculty of Biomedical Sciences, Medical University of Lublin, Chodzki 1, 20-093 Lublin, Poland <sup>5</sup> Institute of Physical Chemistry Polish Academy of Sciences, Kasprzaka 44/52, 01-224 Warsaw, Poland <sup>6</sup> Independent Unit of Tissue Engineering and Regenerative Medicine, Faculty of Biomedical Sciences, Medical University of Lublin, Chodzki 1, 20-093 Lublin, Poland; Department of Amorphous and Structurally Ordered Oxides, Chuiko Institute of Surface Chemistr
11:00-11:10		<b>Low frequency Raman spectroscopy for characterization of amorphous and crystalline variably substituted hydroxyapatites</b> Joshua Kirkham <sup>1</sup> , Tim Kortner <sup>2</sup> , Kārlis Bērziņš <sup>1</sup> , Cushla McGoverin <sup>3</sup> , Keith Gordon <sup>1</sup> , Sara Miller <sup>1</sup> <sup>1</sup> Te Whai Ao – The Dodd-Walls Centre for Photonic and Quantum Technologies and Department of Chemistry, University of Otago <sup>2</sup> Department of Chemistry, Syracuse University, Center for Science and Technology <sup>3</sup> Te Whai Ao – The Dodd-Walls Centre for Photonic and Quantum Technologies, and Department of Physics, University of Auckland
11:15-11:25		<b>Exploring the glycosaminoglycan structure: does it fold and how?</b> Gergo Peter Szekeres <sup>1</sup> , Jan Horlebein <sup>2</sup> , Jerome Riedel <sup>1</sup> , Gert Von Helden <sup>2</sup> , Mark Mero <sup>3</sup> , Kevin Pagel <sup>1</sup> , Zsuzsanna Heiner <sup>4</sup> <sup>1</sup> Freie Universität Berlin, Fritz-Haber-Institut der Max-Planck-Gesellschaft <sup>2</sup> Fritz-Haber-Institut der Max-Planck-Gesellschaft <sup>3</sup> Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy <sup>4</sup> School of Analytical Sciences Adlershof, Humboldt-Universität zu Berlin
11:30-11:40		<b>Phosphine Halogen-Bonded Complexes: Investigated Using Matrix Isolation IR Spectroscopy</b> Elliot Tay <sup>1</sup> , Corentin Grassin <sup>1</sup> , Clemens Müller <sup>1</sup> , Christian Merten <sup>1</sup> <sup>1</sup> Organische Chemie II, Fakultät für Chemie und Biochemie
11:45-11:55		<b>Raman spectroscopy for investigation of interaction within polymer based magnetic multicomponent scaffolds</b> Anna Kołodziej <sup>1</sup> , Małgorzata Świętek <sup>2</sup> , Anna Hlukhaniuk <sup>2</sup> , Daniel Horák <sup>2</sup> , Aleksandra Wesołucha-Birczyńska <sup>1</sup> <sup>1</sup> Faculty of Chemistry, Jagiellonian University <sup>2</sup> Institute of Macromolecular Chemistry, Czech Academy of Sciences
12:00-12:10		<b>Which method will distinguish nanofibrous carbon materials?</b> Aleksandra Wesołucha-Birczyńska <sup>1</sup> , Maria Pajda <sup>2</sup> , Elżbieta Długoń <sup>3</sup> , Krzysztof Morajka <sup>1</sup> , Marek Michalec <sup>1</sup> , Marta Błażewicz <sup>4</sup> <sup>1</sup> Faculty of Chemistry, Jagiellonian University <sup>2</sup> Technolutions <sup>3</sup> AGH – University of Science and Technology, Faculty of Materials Science and Ceramics, <sup>4</sup> AGH – University of Science and Technology, Faculty of Materials Science and Ceramics
	A0-03	<b>(D) Spectroscopy of surface&amp;interfaces</b> Chair: Inez Weidinger
10:45-11:00		<b>Surface-enhanced resonance Raman spectro-electrochemistry as a tool to study redox-related structural changes in (bio)chemistry in-situ</b> Michelle Mahler <sup>1</sup> , Patrycja Kielb <sup>1</sup> <sup>1</sup> University of Bonn
11:05-11:20		<b>Tip-enhanced Raman spectroscopy for nanoscale studying of catalytic. systems</b> Bin Ren <sup>1</sup> , Xiang Wang <sup>1</sup> , Tengxiang Huang <sup>1</sup> , Huishu Feng <sup>1</sup> <sup>1</sup> Xiamen University



11:25-11:35		<b>Mechanistic insights of conjugated acetylenic polymers for the photoelectrochemical nitrogen reduction reaction to ammonia</b> Mino Borrelli <sup>1</sup> , Agnieszka Kuc <sup>2</sup> , Xinliang Feng <sup>1</sup> , Inez Weidinger <sup>1</sup> <sup>1</sup> TUD <sup>2</sup> Helmholtz-Zentrum Dresden-Rossendorf
11:40-11:50		<b>Revealing the Size Effect of Pd/Au Bimetallic Catalysts at Nanoscale with Tip-enhanced Raman Spectroscopy</b> Xiang Wang <sup>1</sup> , Hui-shu Feng <sup>1</sup> , Hai-sheng Su <sup>1</sup> , Ya-qiong Su <sup>2</sup> , Bin Ren <sup>1</sup> <sup>1</sup> Xiamen University <sup>2</sup> Xi'an Jiaotong University
11:55-12:05		<b>The study of correlated Stokes-and-anti-Stokes in normal Raman and in Surface-Enhanced Raman Scattering (SERS)</b> Filomeno Aguiar Junior <sup>1</sup> , Sahar Milani <sup>1</sup> , Sanker Timsina <sup>2</sup> , Stanislav Konorov <sup>1</sup> , Michele L. de Souza <sup>1</sup> , Rogério De Sousa <sup>3</sup> , Alexandre Brolo <sup>1</sup> <sup>1</sup> Department of Chemistry, University of Victoria-BC <sup>2</sup> Department of Physics, University of Victoria-BC <sup>3</sup> Department of Physics, University of Victoria-BC
	A0-01	<b>(H) Biodiagnostic spectroscopy</b> Chair: Michael Heise
10:45-11:00		<b>Raman imaging and AFM studies of human colon tissues and cells – cholesterol impact on CRC development</b> Beata Brozek-Pluska <sup>1</sup> , Karolina Beton-Mysur <sup>1</sup> <sup>1</sup> Lodz University of Technology, Faculty of Chemistry, Laboratory of Laser Molecular Spectroscopy
11:05-11:20		<b>Raman Spectroscopy for Pre-Disease Analysis</b> Pradjna Paramitha <sup>1</sup> , Keita Iwasaki <sup>1</sup> , Kosuke Hashimoto <sup>1</sup> , Bibin Andriana <sup>1</sup> , Hidetoshi Sato <sup>1</sup> <sup>1</sup> Department of Biological and Environmental Sciences, Kwansei Gakuin University
11:25-11:35		<b>Application of Raman spectroscopy to examine tattoo pigments in tissues</b> Katarzyna Karpienko <sup>1</sup> , Aneta Szczerkowska-Dobosz <sup>2</sup> , Patrycja Rogowska <sup>2</sup> , Iwona Kaczmarzyk <sup>1</sup> , Maciej S. Wróbel <sup>1</sup> <sup>1</sup> Department of Metrology and Optoelectronics, Faculty of Electronics, Telecommunication and Informatics, Gdansk University of Technology <sup>2</sup> Department of a Department of Dermatology, Venereology and Allergology, Faculty of Medicine, Medical University of Gdańsk <sup>3</sup> Department of Metrology and Optoelectronics, Faculty of Electronics, Telecommunication and Informatics, Gdansk University of Technology
11:40-11:50		<b>Raman analysis of breast microcalcifications, correlation with pathology</b> Carlo Morasso <sup>1</sup> , Renzo Vanna <sup>2</sup> , Francesca Piccotti <sup>1</sup> , Marta Truffi <sup>1</sup> , Sara Albasini <sup>1</sup> , Thomas Huthwelker <sup>3</sup> , Laura Villani <sup>4</sup> , Oliver Bunk <sup>3</sup> , Cinzia Giannini <sup>4</sup> , Fabio Corsi <sup>5</sup> <sup>1</sup> Istituti Clinici Scientifici Maugeri IRCCS <sup>2</sup> Institute for Photonics and Nanotechnologies, National Research Council (IFN-CNR) <sup>3</sup> Paul Scherrer Institut <sup>4</sup> Institute of Crystallography, National Research Council <sup>5</sup> Department of Biomedical and Clinical Sciences, University of Milan
11:55-12:05		<b>Pre-clinical characterization of Osteopetrosis in Mice Models by Raman microspectroscopy</b> Marco Ventura <sup>1</sup> , Alejandro De La Cadena <sup>1</sup> , Morteza Behrouzitabar <sup>2</sup> , Maria Lucia Schiavone <sup>3</sup> , Federico Vernuccio <sup>2</sup> , Giulio Cerullo <sup>2</sup> , Cristina Sobacchi <sup>3</sup> , Dario Polli <sup>2</sup> , Renzo Vanna <sup>1</sup> <sup>1</sup> CNR-IFN <sup>2</sup> Politecnico di Milano <sup>3</sup> IRCCS Humanitas Research Hospital
12:10-13:10		Lunch
13:10-14:30		SESSION 2
	A1-01	<b>(I) Chemometrics&amp;machine learning</b> Chair: Valeria Tafintseva
13:10-13:20		<b>Long short-term memory and Transformer in Classification and Correction of ATR distorted spectrum</b> Rui Cheng <sup>1</sup> , Johannes Kiefer <sup>1</sup> <sup>1</sup> University of Bremen

13:25-13:35		<b>Classifying Cheddar cheese based on maturity level and manufacturer using vibrational spectroscopy and chemometrics.</b> Gerson R. Dewantier <sup>1</sup> , Peter J. Torley <sup>1</sup> , Ewan W. Blanch <sup>1</sup> <sup>1</sup> RMIT University
13:40-13:50		<b>Characterization of root tissue development associated with lodging tendency in tef using Raman micro-spectroscopy</b> Sabrina Diehn <sup>1</sup> , Noa Kirby <sup>1</sup> , Shiran Ben-Zeev <sup>1</sup> , Yehoshua Saranga <sup>1</sup> , Rivka Elbaum <sup>1</sup> <sup>1</sup> The Robert H Smith Faculty of Agriculture, Food and Environment, Hebrew University of Jerusalem
13:55-14:05		<b>Plasmonic surface enhanced infrared spectroscopy aided with artificial intelligence for structural protein biomarker based neurodegenerative disease detection</b> Deepthy Kavungal <sup>1</sup> , Pedro Magalhães <sup>2</sup> , Senthil Kumar <sup>2</sup> , Rajasekhar Kolla <sup>2</sup> , Hilal Lashuel <sup>2</sup> , Hatice Altug <sup>1</sup> <sup>1</sup> Institute of Bioengineering, EPFL <sup>2</sup> Brain Mind Institute, EPFL
14:10-14:20		<b>The use of NIR spectroscopy for the analysis of Fumonisin B1 (FB1)</b> Anja Laubscher <sup>1</sup> , Paul J. Williams <sup>1</sup> , Lindy J. Rose <sup>1</sup> <sup>1</sup> Stellenbosch University
14:25-14:35		<b>A multivariate surface-enhanced infrared absorption (SEIRA) method based on quantum dots and universal attenuated total reflectance (UATR) accessory for atrazine determination</b> Felipe Trindade <sup>1</sup> , Izabel Souza Sobrinha <sup>1</sup> , Giovannia Pereira <sup>1</sup> , Claudete Pereira <sup>1</sup> <sup>1</sup> Universidade Federal de Pernambuco
	A1-02	<b>(J) Computational approaches</b> Chair: James Cheeseman
13:10-13:25		<b>Raman Optical Activity: Simulations Outside and In Resonance</b> Petr Bour <sup>1</sup> <sup>1</sup> Institute of Organic Chemistry and Biochemistry
13:30-13:45		<b>CHIROPTICAL SPECTRA: WHEN CALCULATIONS MEET THE EXPERIMENT</b> Joanna E. Rode <sup>1</sup> <sup>1</sup> Institute of Nuclear Chemistry and Technology, Dorodna 16
13:50-14:00		<b>A study of synchrotron-based UV-resonance Raman spectra of N-acetylamino saccharides – In combination with their ATR-far ultraviolet spectroscopy study</b> Kousuke Hashimoto <sup>1</sup> , Fatima Matroodi <sup>2</sup> , Mariagrazia Tortora <sup>2</sup> , Barbara Rossi <sup>2</sup> , Yusuke Morisawa <sup>3</sup> , Yukihiro Ozaki <sup>1</sup> , Hidetoshi Sato <sup>1</sup> <sup>1</sup> School of Biological and Environmental Sciences, Kwansei Gakuin University <sup>2</sup> Elettra – Sincrotrone Trieste <sup>3</sup> School of Science and Engineering, Kindai University
14:05-14:15		<b>Vibrational Circular Dichroism of Chiral Crystals: The Interplay of Symmetry and Chirality</b> Sascha Jähnigen <sup>1</sup> , Anne Zehnacker <sup>2</sup> , Rodolphe Vuilleumier <sup>1</sup> <sup>1</sup> Ecole Normale Supérieure <sup>2</sup> Institut des Sciences Moléculaires d'Orsay, Université Paris-Saclay
14:20-14:30		<b>Infrared spectrum, Barrier heights and Density Functional Theory calculations of N-(n-Butyl)-N'-[(p-Chloro phenoxy) acetyl] Urea</b> J Sunil <sup>1</sup> , Kanugula Srishailam <sup>1</sup> , B Venkatram Reddy <sup>2</sup> , G Ramana Rao <sup>2</sup> <sup>1</sup> SR University <sup>2</sup> Kakatiya University
14:35-14:45		<b>Quantitative evaluation of IR and corresponding VCD spectra</b> Thomas Mayerhöfer <sup>1</sup> , Ankit Singh <sup>1</sup> , Jer-shing Huang <sup>1</sup> , Christoph Krafft <sup>1</sup> , Juergen Popp <sup>1</sup> <sup>1</sup> Leibniz Institute of Photonic Technology
	A0-04	<b>(A) Advanced characterization of materials</b> Chair: Ana Batista de Carvalho
13:10-13:20		<b>Raman Confocal Imaging for materials at high temperatures</b> Maciej Bik <sup>1</sup> , Piotr Jeleń <sup>1</sup> , Maciej Sitarz <sup>1</sup> <sup>1</sup> AGH University of Science and Technology, Faculty of Materials Science and Ceramics
13:25-13:35		<b>Automated Quantitative Analysis of (Microplastic) Particles and Fibers down to 1 µm by Raman Microspectroscopy</b> Oliver Jacob <sup>1</sup> , Alejandro Ramírez-Piñero <sup>1</sup> , Natalia Ivleva <sup>1</sup> <sup>1</sup> Chair of Analytical Chemistry and Water Chemistry, Technical University of Munich

13:40-13:50		<b>Investigating Degradation of Poly(vinyl chloride) by Spectroscopic Methods</b> Marwa Saad <sup>1</sup> , Krzysztof Kruczała <sup>1</sup> , Marek Bucki <sup>1</sup> , Karol Górecki <sup>1</sup> , Sonia Bujok <sup>2</sup> , Łukasz Bratasz <sup>2</sup> <sup>1</sup> Jagiellonian University, Faculty of Chemistry, <sup>2</sup> Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences
13:55-14:05		<b>Visualization of Intermolecular Hydrogen Bonding of Poly(<math>\epsilon</math>-caprolactone) during Marine Degradation using Low-frequency Raman Spectroscopy</b> Harumi Sato <sup>1</sup> , Tomoaki Segawa <sup>1</sup> , Kohei Ito <sup>1</sup> , Yota Maruyama <sup>1</sup> , Masahiro Hatayama <sup>1</sup> , Gao Jiacheng <sup>1</sup> <sup>1</sup> Kobe University
14:10-14:20		<b>Imaging of Three-dimensional Molecular Orientation Using FT-IR, Raman, and O-PTIR Microspectroscopies of various samples</b> Tomasz Wrobel <sup>1</sup> <sup>1</sup> Jagiellonian University
	A0-03	<b>(D) Spectroscopy of surface&amp;interfaces</b> Chair: Ahmad Salman
13:10-13:25		<b>Quantifying Large-Scale Structural Changes During pH-Induced Channel Opening of Influenza A M2 using Surface-enhanced Infrared Absorption Spectroscopy</b> Ronja Paschke <sup>1</sup> , Swantje Mohr <sup>2</sup> , Sascha Lange <sup>2</sup> , Adam Lange <sup>2</sup> , Jacek Kozuch <sup>1</sup> <sup>1</sup> Freie Universität Berlin <sup>2</sup> Leibniz-Forschungsinstitut für Molekulare Pharmakologie Berlin
13:30-13:45		<b>Mechanistic insights into the electrosynthesis of chemical feedstocks by in situ Raman and ATR-FTIR spectro-electrochemistry</b> Dr. Khoa H. Ly <sup>1</sup> <sup>1</sup> Fakultät für Chemie und Lebensmittelchemie, Technische Universität Dresden, Andreas-Schubert-Bau, Zellescher Weg 19, 01069 Dresden, Germany
13:50-14:00		<b>Nanoscale hyperspectral imaging of biologically relevant molecules</b> Ewelina Lipiec <sup>1</sup> , Michał Czaja <sup>2</sup> , Anna Chachaj-Brekiesz <sup>3</sup> , Adrian Cernescu <sup>4</sup> , Dhiman Ghosh <sup>3</sup> , Dawid Lupa <sup>1</sup> , Roland Riek <sup>3</sup> , Sara Seweryn <sup>2</sup> , Katarzyna Skirlińska-Nosek <sup>2</sup> , Kamila Sołńska <sup>1</sup> , Anita Wnętrzak <sup>3</sup> , Marek Szymoński <sup>1</sup> <sup>1</sup> Jagiellonian University, Faculty of Physics, Astronomy, and Applied Computer Science, M. Smoluchowski Institute of Physics, Cracow, Poland <sup>2</sup> 1) Jagiellonian University, Faculty of Physics, Astronomy, and Applied Computer Science, M. Smoluchowski Institute of Physics, Cracow, Poland, 2) Jagiellonian University, Doctoral School of Exact and Natural Sciences, Cracow, Poland <sup>3</sup> Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Kraków, Poland <sup>4</sup> Attocube Systems AG, Ellinger Weg 2, 85540 Haar, Germany
14:05-14:15		<b>Nanospectroscopy imaging of the molecule/metal interaction</b> Natalia Piergies <sup>1</sup> , Dominika Święch <sup>2</sup> , Magdalena Oćwieja <sup>3</sup> , Czesława Paluszkiewicz <sup>1</sup> , Wojciech M. Kwiatek <sup>1</sup> <sup>1</sup> Institute of Nuclear Physics Polish Academy of Sciences <sup>2</sup> AGH University of Science and Technology, Faculty of Foundry Engineering <sup>3</sup> Jerzy Haber Institute of Catalysis and Surface Chemistry Polish Academy of Sciences
	A0-01	<b>(H) Biodiagnostic spectroscopy</b> Chair: Josep Sule-Suso
13:10-13:20		<b>Study on the effects of cryoconservation on human platelets</b> Diana E. Bedolla <sup>1</sup> , Gaia Gavioli <sup>2</sup> , Agnese Razzoli <sup>2</sup> , Eleonora Quartieri <sup>3</sup> , Barbara Iotti <sup>3</sup> , Pamela Berni <sup>3</sup> , Giovanni Birarda <sup>4</sup> , Lisa Vaccari <sup>4</sup> , Davide Schioli <sup>3</sup> , Chiara Marraccini <sup>3</sup> , Roberto Baricchi <sup>3</sup> , Lucia Merolle <sup>3</sup> <sup>1</sup> Area Science Park <sup>2</sup> Clinical and Experimental PhD Program, University of Modena and Reggio Emilia <sup>3</sup> AUSL-IRCCS di Reggio Emilia, Transfusion Medicine Unit <sup>4</sup> Elettra Sincrotrone Trieste
13:25-13:35		<b>Fighting peripheral nervous system tumors-hyperspectral imaging as a novel approach to monitor the therapeutic efficacy of cannabidiol</b> Karolina Chrabąszcz <sup>1</sup> , Katarzyna Pogoda <sup>1</sup> , Klaudia Suchy <sup>1</sup> , Agnieszka Panek <sup>1</sup> , Czesława Paluszkiewicz <sup>1</sup> , Wojciech M. Kwiatek <sup>1</sup> <sup>1</sup> Institute of Nuclear Physics, Polish Academy of Science, Krakow, Poland
13:40-13:50		<b>Infrared tissue analysis of Hirschsprung's disease</b> Cymoril Combescot <sup>1</sup> , Anne Durlach <sup>2</sup> , Valérie Untereiner <sup>3</sup> , Francesco Laconi <sup>2</sup> , Olivier Piot <sup>1</sup> <sup>1</sup> University of Reims Champagne Ardenne, BioSpecT <sup>2</sup> Reims University Hospital <sup>3</sup> University of Reims Champagne Ardenne, Cellular and Tissular Imaging

13:55-14:05		<b>Infrared spectral biomarkers of neurodegenerative diseases</b> Lila Lovergne <sup>1</sup> , Dhruva Ghosh <sup>2</sup> , Renaud Schuck <sup>1</sup> , Aris Polyzos <sup>1</sup> , Michael Martin <sup>3</sup> , Edward Barnard <sup>4</sup> , James Brown <sup>5</sup> , Cynthia McMurray <sup>1</sup> <sup>1</sup> Lawrence Berkeley National Laboratory/ Division of Molecular Biophysics and Integrated Bioimaging <sup>2</sup> Lawrence Berkeley National Laboratory/ Department of Statistics <sup>3</sup> Lawrence Berkeley National Laboratory/ Advanced Light Source <sup>4</sup> Lawrence Berkeley National Laboratory/ Molecular Foundry <sup>5</sup> Lawrence Berkeley National Laboratory/ Department of Statistics, and Division of Environmental Genomics and Systems Biology
14:10-14:20		<b>Multimodal spectroscopic imaging of cervical cancer cells exposed to the adaptogenic drug</b> Ewa Pięta <sup>1</sup> , Katarzyna Pogoda <sup>1</sup> , Klaudia Suchy <sup>1</sup> , Karolina Chrabąszcz <sup>1</sup> , Czesława Paluszkiewicz <sup>1</sup> , Wojciech Kwiatek <sup>1</sup> <sup>1</sup> Institute of Nuclear Physics Polish Academy of Sciences
14:25-14:35		<b>FTIR imaging of kidney tissues to diagnose hypertensive organ damage and pharmacological treatment</b> Paola Sassi <sup>1</sup> , Leonardo Pioppi <sup>1</sup> , Niki Tombolesi <sup>1</sup> , Reza Parvan <sup>2</sup> , Gustavo Da Silva <sup>2</sup> , Raffaele Altara <sup>3</sup> , Marco Paolantoni <sup>1</sup> , Assunta Morresi <sup>1</sup> , Alessandro Cataliotti <sup>2</sup> <sup>1</sup> University of Perugia <sup>2</sup> University of Oslo <sup>3</sup> Maastricht University
14:45-15:00	A0-01	SHIM-POL presentation <b>Titel: Nice to have two features in one – the new AIRsight</b> <b>Subject: First measurement results obtained with the new AIRsight. The unique FTIR and Raman Microscope.</b>
18:30 (assembly 17:30)		<b>Conference Dinner</b>
<b>Friday</b>		
9:00-10:15	A0-01	<b>Plenary Session</b>
		Chair: Alexandre Brolo
9:00-9:30		<b>Molecular Optomechanics Approach to Surface-Enhanced Raman Scattering</b> Javier Aizpurua <sup>1</sup> <sup>1</sup> Center for Materials Physics (CSIC-UPV/EHU)
		Chair: Katarzyna Marzec
9:40-10:10		<b>Increasing the utility of infrared spectroscopic imaging by high performance instrumentation and AI</b> Rohit Bhargava <sup>1</sup> <sup>1</sup> Departments of Bioengineering, Electrical & Computer Engineering, Mechanical Science & Engineering, Chemical and Biomolecular Engineering, and Chemistry, Beckman Institute for Advanced Science and Technology, Cancer Center at Illinois, University of Illinois at Urbana-Champaign, 405 N. Mathews Ave., Urbana, IL 61801 USA
10:15-10:45		<b>Coffee Break</b>
10:45-12:10		<b>SESSION 1</b>
	A1-01	<b>(I) Chemometrics&amp;machine learning</b> Chair: Milda Pucetaite
10:45-11:00		<b>In silico experimentation to guide optimization and experimental design in clinical spectroscopy.</b> David Perez-Guaita <sup>1</sup> , Victor Navarro-Esteve <sup>1</sup> , Jaume Bejar-Grimalt <sup>1</sup> , Angel Sanchez-Illana <sup>1</sup> , Hugh J. Byrne <sup>2</sup> <sup>1</sup> University of Valencia <sup>2</sup> Technological University Dublin
11:05-11:20		<b>Sparse Wavelength Sampling in Mid-Infrared Spectroscopy</b> Valeria Tafintseva <sup>1</sup> , Miriam Aledda <sup>1</sup> , Boris Zimmermann <sup>1</sup> , Nageshvar Patel <sup>1</sup> , Volha Shapaval <sup>1</sup> , Achim Kohler <sup>1</sup> <sup>1</sup> Norwegian University of Life Sciences
11:25-11:35		<b>Green Pharmaceutical Quality Control via Infrared Spectroscopy</b> Silke Lehner <sup>1</sup> , Mona Tawab <sup>2</sup> , Holger Latsch <sup>2</sup> , Sandra Ganß <sup>2</sup> , Boris Mizaikoff <sup>3</sup> , Robert Stach <sup>1</sup> <sup>1</sup> Hahn-Schickard <sup>2</sup> Zentrallaboratorium-Deutscher Apotheker <sup>3</sup> Hahn-Schickard

11:40-11:50		<b>Influence of Infrared Imaging measurement modes on breast tissue recognition and cancer diagnosis</b> Danuta Liberda <sup>1</sup> , Tomasz P. Wróbel <sup>2</sup> <sup>1</sup> Jagiellonian University, Doctoral School of Exact and Natural Sciences, Prof. St. Łojasiewicza 11, PL30348, Cracow, Poland <sup>2</sup> Solaris National Synchrotron Radiation Centre, Jagiellonian University, Czerwone Maki 98, 30-92 Krakow, Poland
11:55-12:05		<b>Infrared Diffraction Microtomography of Biological Samples by Solving the Inverse Scatter Problem</b> Eirik Almklov Magnussen <sup>1</sup> , Boris Zimmermann <sup>1</sup> , Uladzislau Blazkho <sup>1</sup> , Simona Dzurendova <sup>1</sup> , Benjamin Dupuy-Galet <sup>1</sup> , Dana Byrtusova <sup>1</sup> , Florian Muthreich <sup>2</sup> , Valeria Tafintseva <sup>1</sup> , Kristian Hovde Liland <sup>1</sup> , Volha Shapaval <sup>1</sup> , Achim Kohler <sup>1</sup> <sup>1</sup> Norwegian University of Life Sciences <sup>2</sup> University of Bergen
	A1-02	<b>(J) Computational approaches</b> Chair: Thomas Mayerhöfer
10:45-10:55		<b>Computing Raman and Raman optical activity spectra for molecules under resonance</b> James Cheeseman <sup>1</sup> <sup>1</sup> Gaussian, Inc.
11:00-11:10		<b>Yes we can! Calculational study of Human Serum Transferrin distinguishes between resonance Raman optical activity and circularly polarized Raman</b> Jonathan Bogaerts <sup>1</sup> , James Cheeseman <sup>2</sup> , Wouter Herrebout <sup>1</sup> , Christian Johannessen <sup>1</sup> <sup>1</sup> University of Antwerp <sup>2</sup> Gaussian Inc.
11:15-11:25		<b>Simulation of vibrational spectroscopies in various environments</b> Vincent Liegeois <sup>1</sup> <sup>1</sup> NISM, Unamur
11:30-11:40		<b>Anharmonicity of amide bands in NIR region – overtones, combinations, structural fingerprint of peptides</b> Justyna Grabska <sup>1</sup> , Krzysztof B. Bec <sup>1</sup> , Christian W. Huck <sup>1</sup> <sup>1</sup> University of Innsbruck
11:45-11:55		<b>Resonance Raman Optical Activity: how to properly measure, correct and simulate spectra</b> Grzegorz Zając <sup>1</sup> , Ewa Machalska <sup>2</sup> , Katarzyna Pajor <sup>3</sup> , Josef Kapitán <sup>4</sup> , Petr Bouř <sup>5</sup> , Malgorzata Baranska <sup>6</sup> <sup>1</sup> Jagiellonian Centre for Experimental Therapeutics (JCET), Jagiellonian University <sup>2</sup> Jagiellonian Centre for Experimental Therapeutics (JCET), Jagiellonian University; Institute of Nuclear Chemistry and Technology <sup>3</sup> Faculty of Chemistry, Jagiellonian University <sup>4</sup> Department of Optics, Palacký University Olomouc <sup>5</sup> Institute of Organic Chemistry and Biochemistry, Academy of Sciences <sup>6</sup> Faculty of Chemistry, Jagiellonian University; Jagiellonian Centre for Experimental Therapeutics (JCET), Jagiellonian University
	A0-04	<b>(A) Advanced characterization of materials</b> Chair: Sagie Katz
10:45-11:00		<b>Operando IR spectroscopic investigations of (hybrid) porous materials</b> Marco Daturi <sup>1</sup> <sup>1</sup> Laboratory of Catalysis and Spectrochemistry, ENSICAEN, UNICAEN, CNRS
11:05-11:20		<b>In situ FTIR, RS and coupled RS/AFM methods for surface understanding of metal oxide materials applied as catalysts for methane abatement</b> Joanna Profic-Paczkowska <sup>1</sup> <sup>1</sup> Faculty of Chemistry Jagiellonian University
11:25-11:35		<b>Structural characterization of amorphous silica coatings combining specular reflectance (SR) and attenuated total reflectance (ATR) infrared spectroscopic techniques</b> Brenda Bracco <sup>1</sup> , Helios Vocca <sup>2</sup> , Silvia Corezzi <sup>2</sup> , Alessandro Di Michele <sup>2</sup> , Laura Silenzi <sup>3</sup> , Angela Trapananti <sup>3</sup> , Flavio Travasso <sup>3</sup> , Stefano Colace <sup>4</sup> , Michele Magnozzi <sup>5</sup> , Paola Sassi <sup>1</sup> <sup>1</sup> Department of Chemistry, Biology and Biotechnology, University of Perugia and Istituto Nazionale di Fisica Nucleare, Sezione di Perugia <sup>2</sup> Department of Physics and Geology, University of Perugia and Istituto Nazionale di Fisica Nucleare, Sezione di Perugia <sup>3</sup> School of Science and Technology – Physics Division, University of Camerino and Istituto Nazionale di Fisica Nucleare, Sezione di Perugia <sup>4</sup> Department of Physics, Università di Genova <sup>5</sup> Department of Physics, Università di Genova, and Istituto Nazionale di Fisica Nucleare, Sezione di Genova



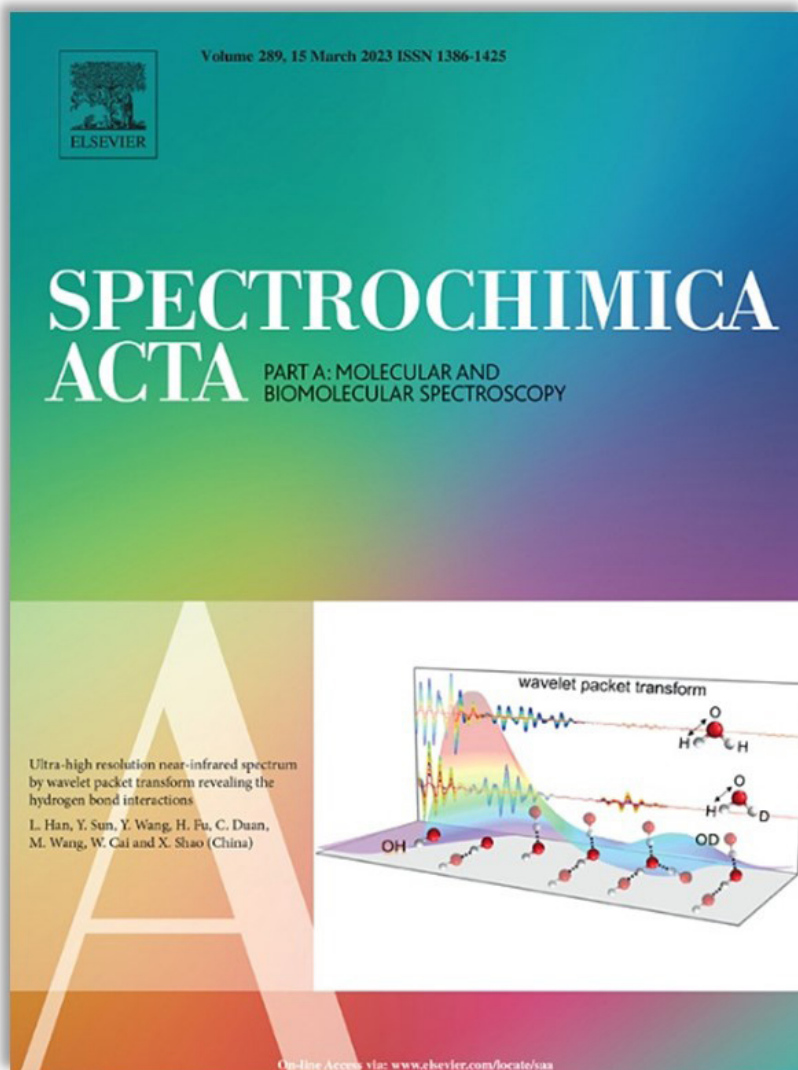
11:40-11:50		<p><b>Can elevated temperatures in HTGR nuclear reactors reverse irradiation damage in graphite? – high-temperature in-situ Raman spectroscopy study</b></p> <p>Magdalena Gawęda<sup>1</sup>, Piotr Jeleń<sup>2</sup>, Małgorzata Frelek-Kozak<sup>1</sup>, Łukasz Kurpaska<sup>1</sup>, Jacek Jagielski<sup>3</sup></p> <p><sup>1</sup>NOMATEN CoE, NOMATEN MAB, National Centre for Nuclear Research</p> <p><sup>2</sup>AGH University of Science and Technology</p> <p><sup>3</sup>National Centre for Nuclear Research, Łukasiewicz Institute for Microelectronics &amp; Photonics</p>
	A0-03	<p><b>(D) Spectroscopy of surface&amp;interfaces</b></p> <p>Chair: Cecilia Spedalieri</p>
10:45-11:00		<p><b>Surface-enhanced Raman Scattering in scaffolds for 3D cell cultures</b></p> <p>Judith Langer<sup>1</sup>, Javier Plou<sup>2</sup>, Clara Clara García-Astrain<sup>1</sup>, Beatriz Molina-Martínez<sup>3</sup>, Luis M. Liz-Marzán<sup>4</sup></p> <p><sup>1</sup>(1) CIC biomaGUNE, Basque Research and Technology Alliance (BRTA), (2) Biomedical Research Networking Center in Bioengineering, Biomaterials, and Nanomedicine (CIBER-BBN)</p> <p><sup>2</sup>(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)</p> <p><sup>3</sup>(1) CIC biomaGUNE, Basque Research and Technology Alliance (BRTA)</p> <p><sup>4</sup>(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</p>
11:05-11:15		<p><b>Spectroscopic study of extracellular vesicles using plasmonic nanoobjects</b></p> <p>Tímea Bebesi<sup>1</sup>, Marcell Pálmai<sup>1</sup>, Anikó Gaál<sup>1</sup>, Imola Csilla Szigyarto<sup>1</sup>, Orsolya Bálint-Hakkel<sup>2</sup>, Zoltán Varga<sup>1</sup>, Judith Mihály<sup>1</sup></p> <p><sup>1</sup>Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences</p> <p><sup>2</sup>Institute of Technical Physics and Material Sciences, Centre for Energy Research</p>
11:20-11:30		<p><b>Giant plasma membrane vesicles as the model systems to resolve nanoscale heterogeneity of native lipid membranes</b></p> <p>Katarzyna Pogoda<sup>1</sup>, Klemencja Berghauzen-Maciejewska<sup>2</sup>, Natalia Piergies<sup>2</sup>, Karolina Chrabąszcz<sup>2</sup>, Czesława Paluszkievicz<sup>2</sup>, Wojciech Kwiątek<sup>2</sup></p> <p><sup>1</sup>Institute of Nuclear Physics Polish Academy of Sciences</p> <p><sup>2</sup>Institute of Nuclear Physics PAN</p>
11:35-11:45		<p><b>SERS based detection of cytosine methylation in genomic DNA</b></p> <p>Stefania D. Iancu<sup>1</sup>, Vlad Moisoiu<sup>1</sup>, Adrian B. Tigu<sup>2</sup>, Andrei Stefancu<sup>1</sup>, Zoltán Bálint<sup>1</sup>, Ciprian Tomuleasa<sup>2</sup>, Nicolae Leopold<sup>1</sup></p> <p><sup>1</sup>Faculty of Physics, Babeş-Bolyai University</p> <p><sup>2</sup>Medfuture Research Center for Advanced Medicine, Iuliu Hatieganu University of Medicine and Pharmacy</p>
	A0-01	<p><b>(H) Biodiagnostic spectroscopy</b></p> <p>Chair: Bayden Wood</p>
10:45-11:00		<p><b>Finding a Needle in a Haystack: Transmission Raman Spectroscopy (TRS) for Detecting Micro Calcifications in Breast Tissue</b></p> <p>Benjamin Gardner<sup>1</sup>, Jennifer Haskell<sup>1</sup>, Adrian Ghita<sup>2</sup>, Charlotte Ives<sup>3</sup>, Douglas Ferguson<sup>3</sup>, Pavel Matousek<sup>4</sup>, Nick Stone<sup>1</sup></p> <p><sup>1</sup>Univeristy of Exeter</p> <p><sup>2</sup>University of Hertfordshire</p> <p><sup>3</sup>Royal Devon University Healthcare NHS Foundation Trust</p> <p><sup>4</sup>STFC</p>
11:05-11:15		<p><b>SERS analysis of urine for prostate cancer detection</b></p> <p>Nicolae Leopold<sup>1</sup>, Stefania D. Iancu<sup>1</sup>, Andrei Stefancu<sup>1</sup>, Vlad Moisoiu<sup>1</sup>, Teodora Telecan<sup>2</sup>, Iulia Andras<sup>2</sup>, Nicolae Crisan<sup>2</sup></p> <p><sup>1</sup>Faculty of Physics, Babeş-Bolyai University</p> <p><sup>2</sup>Urology Department, Iuliu Hatieganu University of Medicine and Pharmacy</p>
11:20-11:30		<p><b>Vibrational spectroscopy for differential diagnosis of patients with rheumatoid and psoriatic arthritis</b></p> <p>Sylwester Mazurek<sup>1</sup>, Izabela Kokot<sup>2</sup>, Agnieszka Piwowar<sup>2</sup>, Renata Sokolik<sup>2</sup>, Monika Kacperczyk<sup>2</sup>, Kamil Rodak<sup>2</sup>, Roman Szostak<sup>1</sup>, Lucyna Korman<sup>2</sup>, Ewa Kratz<sup>2</sup></p> <p><sup>1</sup>University of Wrocław, Department of Chemistry</p> <p><sup>2</sup>Wrocław Medical University</p>

11:35-11:45		<b>Infrared spectroscopy for rapid and objective diagnosis of the etiology of infection as bacterial or viral using a simple peripheral blood test.</b> Ahmad Salman <sup>1</sup> , Uraib Sharaha <sup>2</sup> , Guy Beck <sup>3</sup> , Yotam D. Eshel <sup>3</sup> , Gal Cohen-Logasi <sup>4</sup> , Adam H. Agbaria <sup>5</sup> , Itshak Lapidot <sup>6</sup> , Joesph Kapelushnik <sup>3</sup> , Mahmoud Huleihel <sup>2</sup> , Shaul Mordechai <sup>5</sup> <sup>1</sup> SCE-Sami Shamoon College of Engineering/ Department of Physics <sup>2</sup> Ben-Gurion University/Department of Microbiology, Immunology, and Genetics <sup>3</sup> Soroka University Medical Center/Department of Hematology and Oncology, Saban Pediatric Medical Center <sup>4</sup> SCE-Sami Shamoon College of Engineering/Department of Green Engineering <sup>5</sup> Ben-Gurion University, Department of Physics <sup>6</sup> Afeka Tel-Aviv Academic College of Engineering, Department of Electrical and Electronics Engineering
12:10-12:45	A0-01	<b>Award&amp;Closing Ceremony</b>
12:10-12:20		ICAVS Awards
12:20-12:30		Introduction of ICAVS 13
12:30-12:45		Summary of ICAVS 12 and Good Bye
12:45-13:45		<b>Lunch</b>

# 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 12<sup>th</sup> 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

13:40-14:10 *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, Jagellonian 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  $\mu$ Raman (LabRAM Soleil) and its ParticleFinder<sup>TM</sup> 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: ParticleFinder<sup>TM</sup>: 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

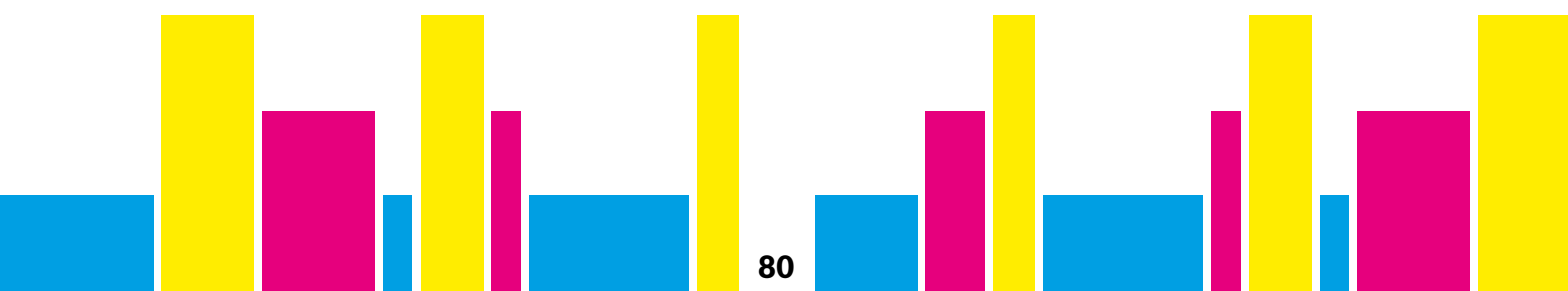
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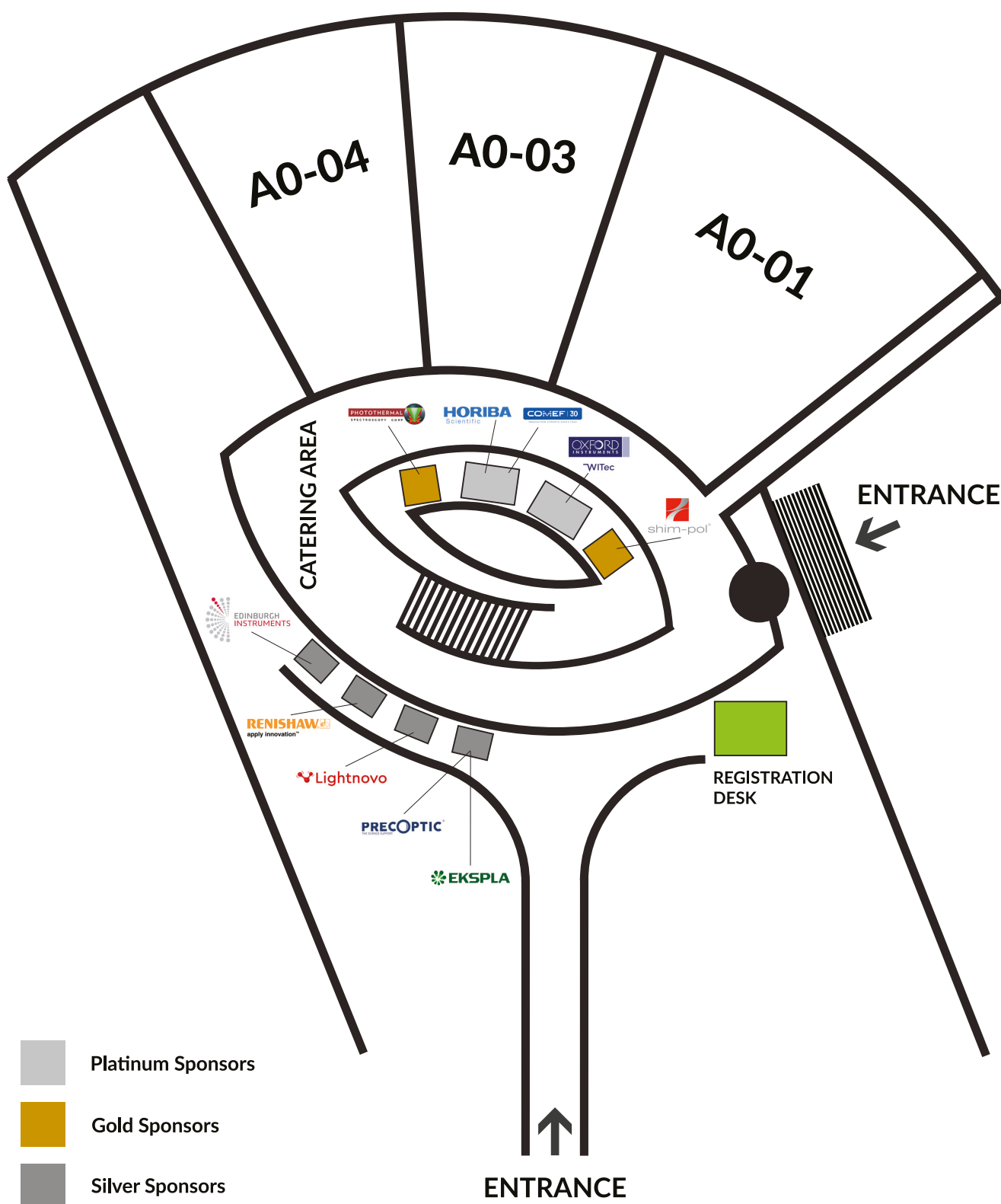
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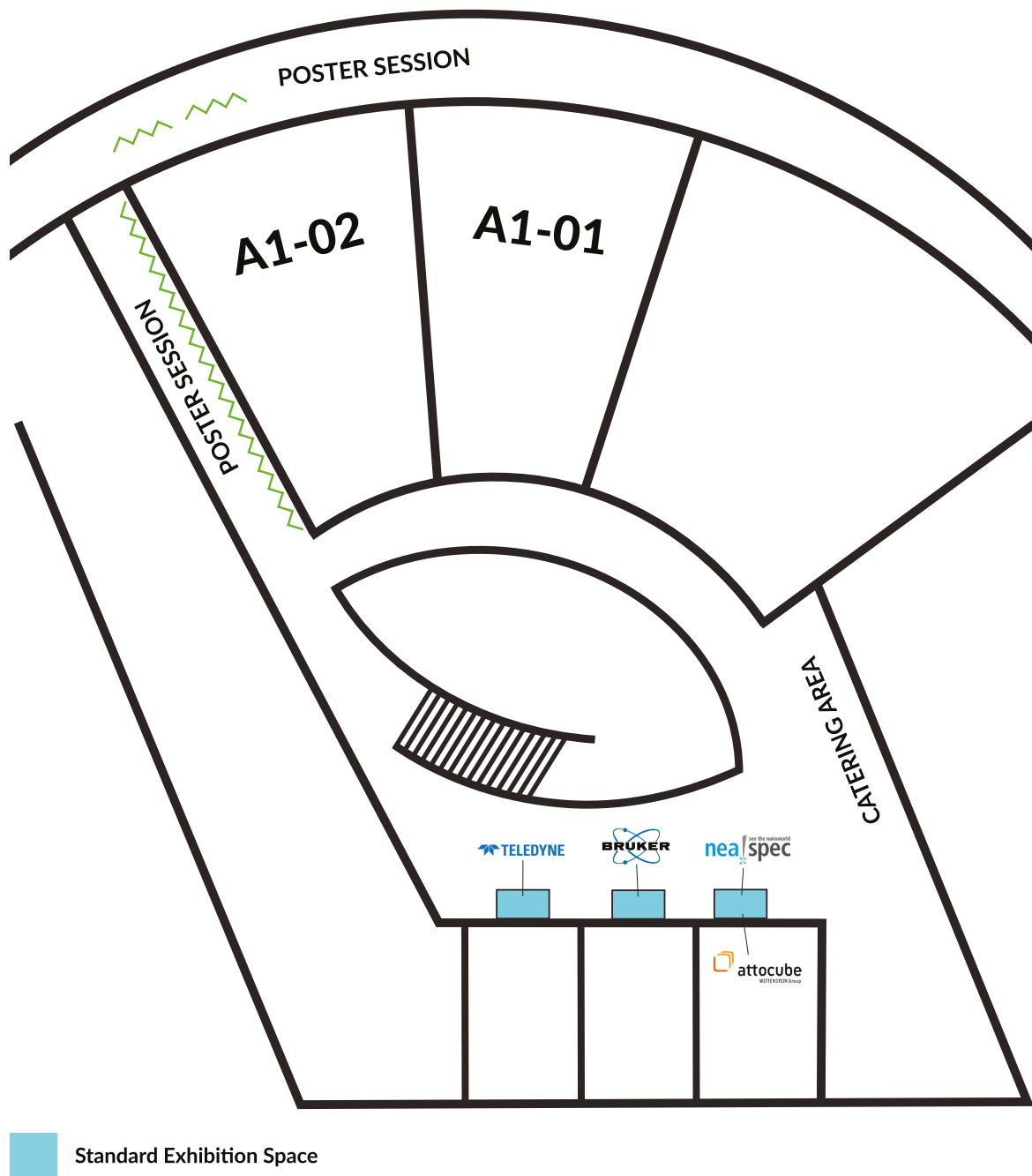




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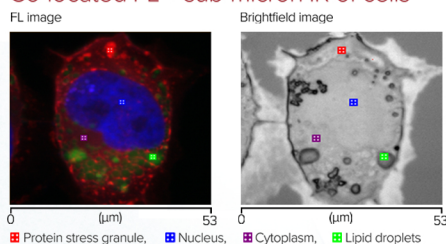
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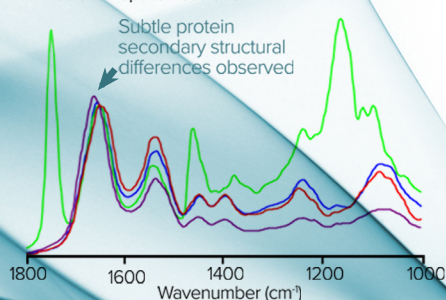


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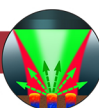
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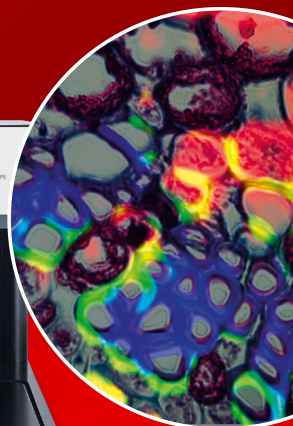
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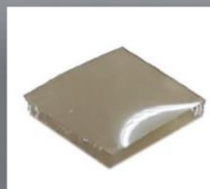
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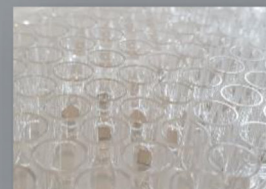
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