TRAINING PROGRAM OF NATURAL PRODUCTS AND DRUG DISCOVERY

24–25 May, 2023
Belgrade, Serbia

Institute for Biological Research "Siniša Stanković"
National Institute of Republic of Serbia (IBISS)
University of Belgrade

TRAINING PROGRAM OF NATURAL PRODUCTS AND DRUG DISCOVERY

24–25 May, 2023
Belgrade, Serbia

SUPPORTED BY

The Training Project of the Alliance of International Science Organizations (ANSO)

CO ORGANIZER BY

Shanghai Institute of Materia Medica, Chinese Academy of Sciences (SIMM)

Institute for Biological Research "Siniša Stanković", National Institute of Republic of Serbia (IBISS), University of Belgrade

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EDITORS

Marina Soković, **Marina Kostić**

GRAPHIC DESIGN

Marija Gačanović Gray

CONTACT

Serbia, **Nađa Hadžimurtović** – panda2020@ibiss.bg.ac.rs

PROGRAMME

Wednesday 24th May

OPENING CEREMONY

09:00-09:30	1. Introduction of guests
	2. Organizer's speech
	3. Group photo

SECTION 1: TRAINING COURSES

09:30-10:15	Machine Learning Integrated Natural Products Chemistry Research	Prof. Yang Ye
10:15-11:00	From TCM to PCSK9 modulator, a way chasing for hypolipidemic candidate	Prof. Lijiang Xuan
11:00-11:15	Coffee break	
11:15-12:00	Discovery and optimization of lead compounds based on new targets	Prof. Bing Zhou
12:00-12:30	Optical Methods for Noninvasive Plant Health Assessment	Dr. Katarina Miletić
12:30-13:30	Lunch	
13:30-14:15	A look back on the emergency drug discovery and development during the COVID-19 pandemic	Prof. Jingshan Shen
14:15-15:00	Preclinical pharmacodynamic evaluation of active compounds against central nervous system diseases	Prof. Haiyan Zhang
15:00-15:15	Coffee break	
15:15-16:00	Pharmacodynamic evaluation of antiviral drugs	Prof. Wei Tang
16:00-16:45	Nonclinical safety evaluation of innovative medicines	Prof. Likun Gong
16:45-17:15	Natural medicinal products: a critical analysis of current and emerging regulatory status in Serbia and Europe	Prof. Miroslav Savić
17:15-17:45	PANDA Council meeting	Council Members

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09:00-09:45	Pharmacokinetic evaluation in early drug discovery stage	Prof. Jia Liu
09:45-10:30	Advanced drug delivery technology for natural product compounds for cancer therapy	Prof. Yongzhuo Huang
10:30-10:45	Coffee break	
10:45-11:15	Bioactive Compounds with Food and Cosmeceutical Applications Derived from Mushrooms and Plant	Dr. Dejan Stojković

SECTION 2: ORAL PRESENTATIONS

11:15-11:30	Pharmacokinetics and metabolism of natural products. The case of oleocanthal, a natural anti-inflammatory agent of olive oil	Dr. Theodora Nikou
11:30-11:45	Natural products: chemistry, bioactivity and application	Dr. Jelena Kukić-Marković
11:45-12:00	Optimizing cordycepin extraction from *Cordyceps militaris* and its determination using high-performance liquid chromatography	Mateja Zotler
12:00-12:15	*Cucumis metuliferus* E. Mey. fruit peel hydro-ethanolic extracts: chemical composition and antibacterial properties	Mladen Rajaković
12:15-12:30	*Foeniculum vulgare* Miller, a New Chemotype from Montenegro	Svetlana Vujović
12:30-13:30	Lunch	
13:30-13:45	The Impact of cytokinins and auxins on biomass and cannabinoid production in callus cultures of cannabis (*Cannabis sativa* L.)	Ana Trajkovska
13:45-14:00	Antioxidant capacity of *Sorbus torminalis* (L.) Crantz and *Viscum album* L.	Toda Ignjatović
14:00-14:15	Comparison of vibrational spectroscopic techniques for determination of phytocannabinoid content in medicinal Cannabis sativa flowers	Olga Gigopulu
14:15-14:45	The Chinese National Compound Library – An open innovation platform	Prof. Dehua Yang
14:45-15:00	Coffee break	

15:00-15:15	General Introduction of SIMM	Prof. Yang Ye
15:15-15:45	Introduction to the international graduate education of SIMM	Prof. Min He
15:45-16:00	Introduction of IBISS	Dr. Mirjana Mihailović
16:00-16:30	Transformation of R&D landscape in Serbia	Prof. Viktor Nedović

GRADUATION CEREMONY

16:30-17:00	1. Speeches by attendee representative
	2. Organizer's speech
	3. Issuing certificates of completion
17:00-17:30	B&R joint laboratory annual meeting

SECTION 1

TRAINING COURSES

Name: YANG YE

Title: Professor

Institution: Shanghai Institute of Materia Medica, Chinese Academy of Sciences

Position: Deputy director, Principal Investigator

E-mail: yye@simm.sc.cn

Machine Learning Integrated Natural Products Chemistry Research

Research Field: Natural Product Chemistry

Abstract: Natural products play an important role in new drug discovery. Discovery and identification of new small-molecule compounds from natural sources have always been an important task in the field of natural product chemistry. With the development of technology, traditional extraction, separation, and structure determination methods have also been continuously updated and improved. In terms of separation, with the advancement of detection and separation techniques, the focus of natural product chemistry has shifted from traditional random separation to systematic and targeted separation of compounds of interest, and constantly challenged the separation and structure determination of trace and ultra-trace natural products. Molecular networking technology based on mass spectrometry and further developed feature-based molecular networking technology are particularly important in avoiding repetitive work and precisely identifying target compounds. Active natural product identification technologies guided by techniques such as ligand fishing, affinity mass spectrometry, and target-based metabolomics can easily select potential bioactive herbs and easily screen candidate compounds in a high-throughput manner, showing great potential in rapidly discovering new drug leading compounds. Our research group has established a platform that combines multiple technologies for the intelligent discovery of natural products, allowing for efficient identification and acquisition of targeted compounds.

Keywords: Natural product, Integrated technology, Machine learning

Short biography: Yang Ye is a full professor of Shanghai Institute of Materia Medica, CAS. He leads a research group focusing on isolation and structural elucidation of bioactive secondary metabolites from medicinal plant resources by establishing a multi-technology platform for quick analysis and separation of natural products. He conducted systematic investigations of commonly used medicinal plants such as the Stemona plants, and provided scientific evidence to explain their traditional therapeutic effects. So far, more than 150 medicinal plants have been investigated, resulting in the identification of 2,500 compounds with more than 1,000 being new. About 20 compounds have developed as candidates for new drug discovery after collaboration with pharmacologists.

Name: LIJIANG XUAN

Title: Professor

Institution: Center of TCM Modernization, Shanghai Institute of Materia Medica, Chinese Academy of Sciences

Position: Principal Investigator

E-mail: ljxuan@simm.ac.cn

From TCM to PCSK9 modulator, a way chasing for hypolipidemic candidat

Research Field: Natural Product Chemistry

Abstract: Hyperlipidemia is the major risk factor of atherosclerosis which can lead to a series of cardiovascular and cerebrovascular diseases and greatly threaten human health. Even though statins have a good efficacy and safety, some medical need is still unmet. Proprotein convertase subtilisin/kexin type 9 (PCSK9) is one of the most promising drug target by far, and its inhibitors or modulators are anticipated to be revolutionary lipid-lowering drugs. Two anti-PCSK9 monoclonal antibodies and one siRNA have already licensed, whereas small molecule inhibitors is still in its initial stage, with both opportunities and challenges.

Traditional Chinese medicine (TCM) often has its unique advantages in the treatment of complicated diseases, especially some cardiovascular and cerebrovascular chronic diseases. Based on TCM theory, hyperlipidemia is related to stasis syndrome, thus there is the potential to discover hits or leads from TCM herbs with stasis-dissolving effects. Based on this hypothesis, we set up a strategy to chase hypolipidemic candidate from TCM with stasis-dissolving function, and series of natural hypolipidemic compounds were discovered with different mode of action on PCSK9 and LDLR.

Keywords: TCM, PCSK9 modulator, LDLR, hyperlipidemia

Short biography: Dr. Lijiang Xuan was graduated from Shanghai Medical University in 1990. In 1995, he obtained Ph.D. degree on Organic Chemistry from Shanghai Institute of Materia Medica, Chinese Academy of Sciences. He has ever worked as a postdoctoral fellow in the department of Pharmaceutical Sciences, Kyushu University, Japan from 1996-1998, and has been a short-term visiting professor in Scripps Institution of Oceanography, USA in 2002-2003. Since 2002, he became a professor in Shanghai Institute of Materia Medica, Chinese Academy of Sciences.

His research interest is focused on drug discovery & development based on chemical and pharmacological investigation of TCM. Till now he has obtained 3 drug licenses in China. Ground on mining of bioactive constituents of Salvia miltiorrhiza, Salvia miltiorrhiza Depsides Salts (SMDS) were developed after series of preclinical and multicentral clinical evaluation on coronary artery disease and chronic angina pectoris. Till now SMDS has been applied to more than 25 million patients. Because of this achievement, Dr. Xuan obtained National Invention Award in China.

Name: BING ZHOU

Title: Professor

Institution: Shanghai Institute of Materia Medica, Chinese Academy of Sciences

Position: Principal Investigator

E-mail: zhoubing@simm.ac.cn

Discovery and optimization of lead compounds based on new targets

Research Field: Discovery and optimization of innovative drugs

Abstract: Discovery of small-molecule drug based on new targets is the trend of medicinal chemistry. However, the efficiency of discovery of lead compounds is still low. To solve this problem, we discover new lead compounds from the following three aspects. 1) We conduct efficient synthetic methodology, build a compound library and expand the chemical space. Then we utilized the high throughput screening and fragment-based drug design to discover lead compounds. 2) We utilized PROTAC technology to design new small-molecule degraders. 3) We carried out structure-based rational drug design to obtained new lead compounds.

Keywords: New targets, efficient synthetic methodology, PROTAC, structure-based rational drug design

Short biography: Dr. Bing Zhou graduated with his Ph.D degree from Shanghai Institute of Materia Medica (SIMM), Chinese Academy of Sciences, and received his postdoctoral training at the Purdue University and the University of Michigan. Now he is a professor and principle investigator of SIMM. Dr. Zhou's laboratory focuses on the discovery and optimization of small-molecule lead compounds, and preclinical candidate selection for further development based on comprehensive druggability evaluation. Dr. Zhou has published over 70 scientific papers on J. Am. Chem. Soc.; Angew. Chem. Int. Ed.; Cancer Res.; J. Med. Chem.; ACS Catal.; Acta Pharm. Sin. B, and other high-impact scientific journals as corresponding, co-corresponding or first author. Over 30 patents have been authorized or filed for application.

Name: KATARINA MILETIĆ
Title: Dr.
Institution: Faculty of Physics Belgrade
Position: Research Assistant
E-mail: katarinamiletic@ff.bg.ac.rs

Optical Methods for Noninvasive Plant Health Assessment

Research Field: Applied physics, biophysics

Abstract: The optical properties of plant leaves can provide valuable information for assessing plant health and detecting early signs of stress and disease. This can be achieved through nondestructive optical methods, such as spectrophotometric measurements, which allow continuous monitoring of the optical transmission coefficients of plant leaves in real-time. Several studies have demonstrated the potential of these methods in detecting nutrient deficiencies, infections of plant pathogens, and monitoring plant health and stress. The proposed methods enable the creation of graphs of spectral circadian rhythms as a function of time, providing insight into the evolution of plant activity over time. In addition to traditional destructive methods, the nondestructive optical methods have been found to be effective in assessing the condition of plants under test. These findings highlight the potential of optical methods in improving plant health assessment and management by providing an early indicator of plant stress and disease, thereby allowing for prompt intervention and treatment. These methods could be particularly useful in hydroponic cultivation, where nutrient deficiencies and stress are common. Overall, the optical properties of plant leaves and nondestructive optical methods hold great promise for improving our understanding of plant responses to growing conditions and promoting successful cultivation of healthy plants.

Keywords: Leaf transmittance, 665 nm red led, Circadian rhythm, plant monitoring, plant health, optical methods

Short biography: Katarina (Milanko) Miletić is a Serbian physicist born on May 30th, 1991, in Čačak. She graduated from a Natural Sciences and Mathematics high school in Čačak in 2010 and went on to pursue a bachelor's degree in Applied and Computer Physics at the University of Belgrade's Faculty of Physics, where she graduated in 2014 with an average grade of 9.52 out of 10. She continued her studies at the same faculty, completing a master's degree in Applied and Computer Physics in 2014 and defending her thesis with a perfect grade of 10.00. Katarina began her doctoral studies in Applied Physics at the University of Belgrade's Faculty of Physics in 2015, receiving scholarships from the Ministry of Education, Science, and Technological Development and the Dositeja Fund for Young Talents. Since 2014, she has been working as a teaching assistant at the Faculty of Physics and the Faculty of Physical Chemistry, where she conducts laboratory and computer exercises for various

courses. Katarina has also led the project 5780 Nondestructive optical method for plant overall health evaluation, which was funded by the Innovation Fund of the Republic of Serbia from September 2020 to December 2021. On August 30th, 2022, she successfully defended her doctoral dissertation titled "Application of Nondestructive Optical Methods in the Assessment of Plant Health and Metabolism." Katarina's dedication to research and teaching in the field of Applied Physics is remarkable and has earned her numerous accolades.

Name: SHEN JINGSHAN

Title: Professor

Institution: Shanghai Institute of Materia Medica, Chinese Academy of Sciences

Position: Principal Investigator

E-mail: shenjingshan@simm.ac.cn

A look back on the emergency drug discovery and development during the COVID-19 pandemic

Research Field: Drug Discovery; Green and Sustainable Chemistry

Abstract: During the global crisis of the outbreak of COVID-19 in early 2020, an emergency teamwork for anti-viral drug discovery was immediately organized in SIMM to find the safe and effective therapeutics against COVID-19. As results of the teamwork, two novel drugs, XIANNUOXIN® (Simnotrelvir Tablets/Ritonavir Tablets (co-packaged)) and MINDVY® (VV116) both were conditional approved for adults suffering from mild to moderate COVID-19 on January 28, 2023 in China. Simnotrelvir targets 3CL protease that is essential for SARS-CoV-2 viral replication; while VV116 targets RNA-dependent RNA polymerase (RdRp) of the virus. A look back on this emergency research is presented.

Keywords: Emergency drug discovery, anti-viral drug, COVID-19 pandemic, Mindvy, Xiannuoxin

Short biography: Prof. Shen completed his undergraduate education at China Pharmaceutical University in 1995 and received a Ph.D. in Organic Chemistry at SIMM in 1998. He is now a Principal Investigator and Ph.D. student advisor at SIMM.

Among the drug discovery projects in his group, VV116 and VV934 were launched in China as anti-SARS-CoV-2 medicines, and VV116 and TPN171 were launched in Uzbekistan for the treatment of COVID-19 and erectile dysfunction (ED) respectively. Six other drug candidates are in different stages of clinical or pre-clinical research.

Shen has gained rich experience in industrial-oriented research and manufacturing. Shen's group proposed a practical concept of "Control from the Route Design" in organic process research and development. They designed and controlled from the very beginning (at the R&D stage) of a project with the principles of Green & Sustainable Chemistry to achieve safer, easier, environment friendly, and cost-efficient process for industrial application.

Name: HAIYAN ZHANG

Title: Professor

Institution: Shanghai Institute of Materia Medica, Chinese Academy of Sciences

Position: Principle Investigator

E-mail: hzhang@simm.ac.cn

Preclinical pharmacodynamic evaluation of active compounds against central nervous system diseases

Research Field: Neuropharmacology

Abstract: Central nervous system diseases can arise from a complex variety of ischemic, hemorrhagic, neurodegenerative, inflammatory, and developmental disorders. Although great progresses have been achieved recently on understanding the pathogenesis of these diseases along with the advanced techniques, there are still vast demands in the discovery of effective central nervous system drugs/drug candidates with the fact of very limited clinical therapeutic strategies. This lecture mainly focuses on introducing the preclinical evaluation of active compounds against various central nervous diseases especially Alzheimer's diseases and ischemic stroke, including representative phenotypic screening and target-based screening methods, assessment of cognitive/psychiatric behavioral changes in animal models of central nervous system diseases, as well as study on pharmacological mechanisms of active compounds.

Keywords: Alzheimer's disease, Ischemic stroke, Phenotypic screening, Behavioral assessment

Short biography: Haiyan Zhang, Ph.D, professor and principle investigator in Shanghai Institute of Materia Medica, Chinese Academy of Sciences. She got her Ph.D degree in Shanghai Institute of Materia Medica, Chinese Academy of Sciences. She had about four years' postdoctoral experience in United States. Her major research interest is discovery of novel therapeutic strategies for Alzheimer's disease (AD), ischemic stroke (IS), and depression, applying three research strategies—natural product-directed, clinical drug-directed and key therapeutic target-directed. Through extensive collaboration with chemistry groups, her research group has currently discovered many novel compounds targeting on various therapeutic targets (AChE, GSK-3β, β-secretase, Aβ aggregation, etc.) or disease-associated key phenotypic changes of AD, IS or depression. Her research group has published over 100 scientific articles in SCI-cited journals, and obtained over 20 invention patent licenses.

Name: WEI TANG

Title: Professor

Institution: Infectious Disease Research Center, Shanghai Institute of Materia Medica, Chinese Academy of Sciences

Position: Principal Investigator

E-mail: tangwei@simm.ac.cn

Pharmacodynamic evaluation of antiviral drugs

Research Field: Dedicating on the drug discovery and evaluation for treatment of autoimmune diseases (psoriasis, IBD, nephritis, et al), viral infectious diseases (DV, Flu, CoV et al) and exploring their mechanisms of pharmacological action.

Abstract: Despite the intensive understanding of virus pathogenesis, and innovative techniques applied to drug research, only a few antiviral drugs have been developed for wide clinical use to prevent or treat infection. There is a great need for more antiviral drug with diverse target mechanisms. Here, we introduce the classical techniques in antiviral drug evaluation, and highlight the progress of some gold standard assays with the developing of modified techniques. Based on the established assay system, we evaluate the anti-ZIKV effect of Hemin *in vitro* and explore the underlying mechanism focus on the virus life cycle and functions of the host cell.

Keywords: Antiviral, Screening, Cell-based, Pharmacodynamic Evaluation, Mechanism

Short biography: Dr. Tang has been working in Shanghai Institute of Materia Medica (SIMM), Chinese Academy of Sciences (CAS), since she got her PhD degree in 2005. She focuses on the drug discovery for the treatment of autoimmune diseases and viral infectious diseases, and exploring their mechanisms of pharmacological action. After successfully formed a highly efficient screening and evaluation system both *in vitro* and *in vivo*, several drug candidates have been found and are currently in the advanced stages of clinical development. She has published more than 80 research articles in SCI journals and obtained more than 20 authorized invention patents. She was elected as a "Young leading talent of scientific and technological innovation" from the Ministry of Science and Technology of China.

Name: LIKUN GONG

Title: Professor

Institution: Shanghai Institute of Materia Medica, Chinese Academy of Sciences

Position: Principal Investigator, Associate Director of Center for Drug Evaluation and Research (CDSER), SIMM

E-mail: lkgong@cdser.simm.ac.cn

Nonclinical safety evaluation of innovative medicines

Research Field: Pharmacology and toxicology

Abstract: Up to now, SIMM has built and improved a preclinical safety evaluation platform that complies with international multilateral GLP regulations, as well as the key technologies and regulatory specifications for toxicity evaluation of different drugs, such as small molecule compounds, biologics, cell and gene therapy products. In addition, case studies were summarized to illustrate the role of early safety testing/screening and nonclinical GLP Toxicological studies in the research and development of innovative medicines in Center for drug safety evaluation and research in SIMM.

Keywords: Nonclinical, safety evaluation, innovative medicines

Short biography: Professor Likun Gong is a PI in the Translational Drug Safety with more than 20 years of experience. She received the PhD in pharmacology in 2005. She then did post-doctoral hepatic drug transporter research at the Tokyo university in Japan. In 2000 she joined SIMM where she worked as the toxicologist on drug safety evaluation and lead a team responsible for early toxicity screening and molecular toxicology research. Her role has gradually broadened to cover all aspects of preclinical safety evaluation studies such that she now leads the non-clinical safety strategy at CDSER, SIMM. She has published over 100 articles in this field. Her team has been built and improved a preclinical safety evaluation key technology that conforms to the international ICH guidelines and complying with international multilateral GLP regulations. She had led the team to complete nearly 100 NMPA IND approved/listed new drug candidates, and more than 50 international IND filings.

Name: MIROSLAV SAVIĆ
Title: PhD
Institution: University of Belgrade – Faculty of Pharmacy
Position: Full Professor
E-mail: miroslav@pharmacy.bg.ac.rs

Natural medicinal products: a critical analysis of current and emerging regulatory status in Serbia and Europe

Research Field: Drug Discovery and Development; Pharmaceutical Regulation

Abstract: Unlike natural products used as animal feeds, food supplements or cosmetic products, the regulation of such products as medicinal products is generally expected to be fully compliant with the legislation for all other products approved for the prevention or treatment of disease. In this sense, they must meet the requirements to ensure the declared quality, adequate safety and efficacy characteristic of medicinal products. Accordingly, advertising medicines to the public by claiming that their safety or efficacy is due to the fact that they are natural is legally prohibited. However, in some cases, certain adjustments are made to the regulations. In particular, the pharmacological effects or efficacy of traditional herbal medicines are only plausible based on many years of use and experience. Such use for certain indications without clear evidence from clinical trials makes this subtype of natural medicines a kind of borderline product. The legal existence of natural product categories that do not have to meet all the criteria for medicinal products poses a challenge. Namely, an adequately tested product should be either a medicinal product that works or a non-medicinal product that may or may not work, the latter of which may ultimately lead to misuse of some products.

Keywords: Medicinal products, natural medicinal products, evidence, traditional medicinal products

Short biography: Miroslav M. Savić is professor of Pharmacology and Pharmacotherapy at the University of Belgrade – Faculty of Pharmacy. The primary field of his scientific research is neuropsychopharmacology. He is mentor of 12 PhD theses defended, and authored 92 Scopus/PubMed cited publications in peer reviewed international and national scientific journals, with h-index of 24. He has long-term fruitful collaboration with research groups from USA, Austria and Canada. Within a H2020-Innovative Medicines Initiative project, he was a leader of work package devoted to improving the preclinical prediction of psychiatric adverse effects. He is co-inventor of two international patents related to discovery of novel ligands that act selectively at distinct subtypes of GABAA receptors. He was project coordinator of two national projects granted by Ministry of Education, Science and Technological Development of Republic of Serbia, and currently leads a project funded by the National fund of Serbia. His professional engagement in the public health system of Serbia is related to regulation of registration and clinical trials of medicines, as a full-member of the Commission for registration of human medicines of the Medicines and Medical Devices Agency of Serbia and the Ethics Committee of Republic of Serbia, respectively.

Name: JIA LIU

Title: Professor

Institution: Shanghai Institute of Materia Medica, Chinese Academy of Sciences

Position: DMPK Center

E-mail: jia.liu@simm.ac.cn

Pharmacokinetic evaluation in early drug discovery stage

Research Field: Drug metabolism and pharmacokinetics

Abstract: In drug development, the evaluation of drug efficacy during the drug development process is crucial. It is an important task of drug metabolism to obtain as effective evaluation results as possible in the early stage of drug discovery under limited funding support and to use these evaluation results to guide further modification. In this report, the basic evaluation strategy and basic structural modification ideas of Shanghai Institute of Materia Medica will be introduced. The significance and value of each experiment in further evaluation will be discussed with the aim of achieving high output evaluation.

Keywords: Pharmacokinetic evaluation

Short biography: Dr. Liu Jia, an analytical chemist at the Shanghai Institute of Materia Medica, Chinese Academy of Sciences, focuses on drug metabolism and metabolomics utilizing mass spectrometry-based techniques. Her research involves developing analytical methodologies, studying drug metabolism mechanisms, evaluating the efficacy of Chinese medicine, and examining the function of endogenous metabolites in disease progression and drug intervention. Dr. Liu has published 19 research articles in well-regarded scientific journals, including Analytical Chemistry, Analytica Chimica Acta, Acta Pharmacologica Sinica, Gut Microbes, and Nature Communications, as either the corresponding or first author. Her extensive experience in drug evaluation encompasses over 5,000 drug-like property assessments of lead compounds, 100 pre-clinical studies of *in vitro* metabolism, and drug-drug interactions, three pre-clinical pharmacokinetic-pharmacodynamic (PKPD) studies of innovative drugs, four pre-clinical pharmacokinetic and drug metabolism analyses of innovative drugs, and six clinical pharmacokinetic assessments of innovative drugs, two of which have been approved for marketing.

Name: Yongzhuo Huang

Title: Professor

Institution: Shanghai Institute of Materia Medica, Chinese Academy of Sciences

Position: Principal Investigator

E-mail: yzhuang@simm.ac.cn

Advanced drug delivery technology for natural product compounds for cancer therapy

Research Field: Pharmaceutics

Abstract: Natural products are a useful source for having lead compounds for drug development. There are a lot of active compounds derived from Chinese traditional medicines demonstrated with therapeutic activities. Yet, the herb-sourced compounds usually have relatively mild activities compared to the synthetically optimized compounds. The potential value for clinical translation can be improved by using advanced pharmaceutical technology for increasing potency via enhancing drug delivery to the pathological sites. In addition, there are the common problems for many natural compounds, such as poor water solubility, instability, and low bioavailability. A proper formulation will be useful to improve the drug ability of these active compounds.

Keywords: Natural compounds, drug delivery, formulation, cancer therapy

Short biography: Prof. Huang obtained his Ph.D. from Zhejiang University and completed postdoc training at the University of Michigan College of Pharmacy. He has been endorsed by the prestigious Outstanding Young Investigator program of National Natural Science Foundation of China (NSFC).

Prof. Huang focuses on application of drug delivery technology, including nanotechnology-based biomaterials and carriers (e.g., liposomes, proteins, synthetic polymers, polysaccharides, exosomes), targeted delivery, transdermal delivery, inhaled delivery.

He has published over 150 SCI articles, with h-index of 48, including 12 featured as front or back covers. He serves as an Associate Editor of International Journal of Pharmaceutics, and is an editorial board member of some high-profile journals, such as Nano Letters, Journal Controlled Release, Acta Pharmaceutica Sinica B, Cancer Biology & Medicine, Medicine in Drug Discovery.

Name: DEJAN STOJKOVIĆ

Title: Dr.

Institution: Institute for Biological Research "Siniša Stanković", National Institute of the Republic of Serbia, University of Belgrade

Position: Associate research professor

E-mail: dejanbio@ibiss.bg.ac.rs

Bioactive Compounds with Food and Cosmeceutical Applications Derived from Mushrooms and Plant Industrial By-Products

Research Field: Biological activity; plants and fungi; ethnopharmacology; chemistry of natural products; food science and by-products

Abstract: Fungi are diverse group of organisms growing on different substrates and are able to produce different chemical structures of interest to biomedical and biotechnological industries. Mushrooms are a promising resource for the food industry due to their potential as a source of bioactive compounds. These bioactive compounds have potential applications in the development of functional foods, nutraceuticals, and cosmeceuticals.

Globally, 30% of the food produced annually is wasted, resulting in substantial economic, environmental, and social costs. The food sector alone generates between 25% and 30% of this waste, with fruits and vegetables' discarded parts accounting for a significant proportion. These waste materials have significant potential for recycling through advanced conversion techniques, leading to the production of sustainable resources like energy, fertilizers, materials, and molecules. Valorizing residues and agri-food by-products is now considered a necessity as well as an opportunity to create high-value products that can have a significant impact on the industrial sector's economy.

This study examines the use of various mushrooms and plant by-products to obtain bioactive compounds. The results show that these products are a rich source of phenolic compounds with bioactive properties that can be effectively incorporated into food matrices and as cosmeceuticals.

Keywords: plant, by-products, mushrooms, bio-waste, industrial applications

Short biography: Dr. Dejan Stojković is a highly accomplished researcher with expertise in the field of biological activity, plants and fungi, ethnopharmacology, chemistry of natural products, food science and by-products. He is a senior research associate with over 15 years of experience in the field of bioactivities of natural products. He earned his Ph.D. from the University of Belgrade, Serbia, where he also completed his undergraduate studies in chemistry.

Throughout his academic career, Dr. Stojković has focused on the study of natural products, specifically plants and fungi, to identify their potential biological activity and ethnopharmacological uses. Dejan's research has centered on discovering natural products with potential medicinal properties,

particularly those with antimicrobial, anti-inflammatory, antioxidant, and anticancer activities. His research has contributed to the development of new therapeutic agents and has been published in numerous high-impact journals. In addition to his expertise in natural product chemistry, he has also conducted research in the field of food science and by-products, with a focus on sustainable and efficient use of food waste. Dr. Stojković is serving as an associate editor in numerous scientific journals.

Dr. Stojković has been cited more than 2500 times, with h-index of 34 according to Google scholar database.

SECTION 2

ORAL PRESENTATIONS

Name: THEODORA NIKOU

Title: Dr.

Institution: Department of Pharmacy, National and Kapodistrian University of Athens

Position: Research Associate

E-mail: th-nikou@pharm.uoa.gr

Pharmacokinetics and metabolism of natural products. The case of oleocanthal, a natural anti-inflammatory agent of olive oil

Research Field: Natural products metabolism

Abstract: Olive oil (OO) has been established in public consciousness as a superior edible oil, due to its exceptional nutritional value and sensory properties, mainly attributed to its chemical composition. Apart from fatty acids, OO contains also a highly complex and variable mixture of relative polar compounds, known as OO biophenols. OO biophenols have been extensively studied for their biological and pharmacological properties. However, limited data exist for their metabolic fate *in vivo*, a commonly underestimated aspect in natural products research. Oleocanthal (Oleo) is one of these biophenols, acting as a strong inti-inflammatory agent, while studies have also shown its antioxidant and antimicrobial properties. Though, its pharmacokinetic properties have never been described so far. Towards this purpose, Oleo was isolated in high amount and purity from OO and administered to a mouse-model. A pharmacokinetic experiment was designed and Oleo was supplemented in the dose of 5 mg/kg in a mice model. Plasma samples were collected in ten time points and analyzed via LC-HRMS/MS. The pharmacokinetic characteristics of Oleo and its metabolic derivatives were determined in time, along with their relative content. Novel biomarker compounds were revealed and associated for the time with Oleo administration.

Keywords: Natural products, metabolism, pharmacokinetics, olive oil, oleocanthal

Name: JELENA KUKIĆ-MARKOVIĆ
Title: PhD
Institution: University of Belgrade – Faculty of Pharmacy
Position: Assistant Professor
E-mail: jelena.kukic@pharmacy.bg.ac.rs

Natural products: chemistry, bioactivity and application

Research Field: Pharmacognosy; Phytotherapy

Abstract: The focus of research group from Department of Pharmacognosy at the Faculty of Pharmacy in Belgrade is on natural products, their chemistry and application. Main subjects of research are analysis of composition and bioactivities of various plant isolates (extracts, essential oils), isolation and structural analysis of active specialized plant metabolites, optimization of extraction procedures involving new techniques, and green chemistry principles. Since the Balkan Peninsula is one of the centers of plant biodiversity, our main objective is to explore the autochthonous taxa, especially endemic and rare ones, in terms of their distribution, conservation, morphology, chemistry, pharmacology and potential utilization. The main outcomes of these studies are the identification of new herbal raw materials and isolates, their pharmacognostic and pharmacological characterization, and the development of methods of quality assessment and evaluation of safe use of natural products, along with exploring other ways of their use. Important segment of research focuses on identifying natural principles and influences on secondary plant metabolism and studying the chemotaxonomic potential of certain plant metabolites. Basic research interest of this group is constantly upgraded trough scientific collaboration with colleagues from other research institution from Serbia, neighboring regions and abroad, resulting in many scientific and professional publications, and PhD theses.

Keywords: Natural products, plant isolates, chemistry, bioactivity

Name: MATEJA ZOTLER
Title: Student
Institution: Mycomedica Ltd, Slovenia
Position: Researcher
E-mail: lab@goba.eu

Optimizing cordycepin extraction from *Cordyceps militaris* and its determination using high-performance liquid chromatography

Research Field: Analytical Chemistry

Abstract: *Cordyceps militaris* is a medicinal fungus highly valued in traditional Asian medicine, with its main bioactive compound being cordycepin. The aim of my research was to optimize the extraction of cordycepin from dried and powdered *C. militaris*. For monitoring the efficiency of the extraction, I partially validated an HPLC analytical method for determining cordycepin in extracts. I approached the optimization through single-factor experiments. Each parameter was optimized in a separate series of experiments, where the parameter of interest was varied while keeping the other parameters constant. The optimized value of the parameter was then used in further series of experiments. The extraction efficiency was evaluated based on the optimal ratio of cordycepin extracted and the percentage of impurities in the dry extract. In my research, I conducted 5 major groups of experiments, studying the influence of: the ethanol concentration in the solvent on the extraction efficiency, different ratios of solvent volume to dry sample mass on the extraction efficiency, leaching of cordycepin from a sample from which the extract was sequentially removed and fresh solvent added, pH of the sample-solvent mixture on the extraction efficiency, and percolation at different temperatures.

Keywords: Extraction, *Cordyceps militaris*, optimization of process, HPLC

Name: MLADEN RAJAKOVIĆ

Title: PhD student (Master of Science in Biochemistry)

Institution: Institute for Biological Research "Siniša Stanković", National Institute of the Republic of Serbia, University of Belgrade

Position: Junior research assistant

E-mail: mladen.rajakovic@ibiss.bg.ac.rs

Cucumis metuliferus E. Mey. fruit peel hydro-ethanolic extracts: chemical composition and antibacterial properties

Research Field: Phytochemicals; bioanalytical and organic chemistry; drug research and applications; pharmaceutical, agricultural and food Industry; plant cultivation

Abstract: Following the growing trend of circular economy, the focus of our study was the solid/liquid extraction of lyophilized fruit peels of *Cucumis metuliferus* E. Mey. (Cucurbitaceae) under different conditions such as the power of ultrasonic bath (%), ethanol/water ratio (%) and extraction time (min). The percentage yields of the dry extracts varied between 26.37% and 43.98% under different extraction conditions, while the optimal extraction conditions for highest yield were as follows: EtOH (%): 50; Amplitude (%): 40; Time (min): 30. In addition, UHPLC-QToF-MS analysis was performed to determine the chemical composition of 25 different ethanolic and hydro-ethanolic extracts, revealing the presence of the following compounds: dihydroxybenzoic acid, *p*-hydroxybenzoic acid, galloyl pentoside, hydroxybenzoyl hexoside, dihydroxybenzoyl pentoside, vanilloyl hexoside and hydroxybenzoyl rhamnosyl hexoside. The antibacterial properties of these extracts were also tested, and it was discovered that the most effective extracts against the PAO1 strain of *P. aeraginosa* had MBC and MIC values of 0.5 mg/ml and 0.25 mg/ml, respectively. Considering the optimization of extraction conditions of the *C. metuliferus* peels, as well as chemical identification of bioactive compounds present in the extracts, our future research will focus on the bioactive properties of the obtained extracts and their incorporation into food matrices.

Keywords: Kiwano (*Cucumis metuliferus*) peels, extraction, phytochemicals, antibacterial

Name: SVETLANA VUJOVIĆ

Title: pharmD

Institution: Institute for Medicines and Medical Devices of Montenegro

Position: pharmacovigilance associate

E-mail: svetlana.vujovic@cinmed.me

Foeniculum vulgare Miller, a New Chemotype from Montenegro

Research Field: Pharmacognosy

Abstract: Chemical characterization of essential oil obtained from different plants and their different parts is the subject of numerous studies. In this research, a fractionated hydrodistillation extraction procedure was applied to ripe fruit material of fennel, *Foeniculum vulgare* Miller (Apiaceae), collected from three localities in Montenegro: Podgorica, Nikšić, and Kotor. A total of 12 essential oil (EO) samples were obtained from this three localities.

The obtained essential oil samples were analyzed by Gas Chromatography/Mass Spectrometry and Headspace-Gas Chromatography/Mass Spectrometry techniques to characterize the volatile chemical composition of both liquid and vapor phases, and and 18 compounds have been identified.

The phenylpropanoids anethole and estragole and the monoterpenoids α-terpineol and fenchone could be highlighted as the main compounds.

Anethole, estragole and fenchone were the main compounds in the essential oil samples from Podgorica. On the other hand, essential oil samples from Nikšić and Kotor revealed the predominance of fenchone and α-terpineol with a significant amount of anethole. Whereas the samples from Kotor are quite rich in anethole, the ones from Nikšić are characterized by the prevalence of the monoterpene fraction. Accordingly, this chemical profile rich in α-terpineol could represent a new chemotype of fennel essential oil.

Keywords: *α*-terpineol, anethole, fenchone, essential oil, *Foeniculum vulgare Miller*

Name: ANA TRAJKOVSKA

Title: Phd Student

Institution: Faculty of Pharmacy, Ss. Cyril and Methodius University, Skopje

Position: Teaching Assistant

E-mail: ana.trajkovska@ff.ukim.edu.mk

The Impact of cytokinins and auxins on biomass and cannabinoid production in callus cultures of cannabis (*Cannabis sativa* L.)

Research Field: Plant tissue culture, micropropagation, natural products

Abstract: This study evaluated the influence of cytokinin thidiazuron (TDZ) and various auxins such as indole-3-butyric acid (IBA), 2,4-dichlorophenoxyacetic acid (2,4-D) and 1-naphthaleneacetic acid (NAA) on biomass accumulation and cannabinoid production in callus cultures of cannabis (*Cannabis sativa* L.).

Callus cultures were obtained on MS/B5 medium supplemented with 1.0 mg/L TDZ and various concentrations (0.1, 0.5 and 1.0 mg/L) of IBA, 2,4-D and NAA. The DAB Pharmacopoeial method for Cannabis flos was used for quantification of cannabinoids in calli and the results were expressed as µg/g dry extract (DE).

Two main cannabinoids denoted as cannabidiolic acid (CBDA) and tetrahydrocannabinolic acid (THCA) were identified and quantified in callus extracts. The MS/B5 medium with 1.0 mg/L TDZ and 0.5 mg/L IBA was noticed as the most favorable combination of phytohormones for biomass accumulation (17.56 g) and CBDA production (5.53 µg/g DE). The production of CBDA did not give clear cut answer in the presence of various concentrations of auxins 2,4-D (3.08-4.46 µg/g DE) and NAA (2.69-3.31 µg/g DE). The lowest used concentration (0.1 mg/L) of all tested auxins enhanced the production of THCA. The THCA production was significantly increased in calli cultured in the presence of 0.1 mg/L IBA (32.3 µg/g DE) in comparison with those cultured on 0.1 mg/L 2,4-D and NAA (18.32 and 18.15 µg/g DE, respectively).

Cannabis callus cultures represent an efficient biotechnological system for continuous production of bioactive compounds including cannabinoids.

Keywords: Auxins, *Cannabis sativa* L., cannabinoids, cytokinins, callus cultures

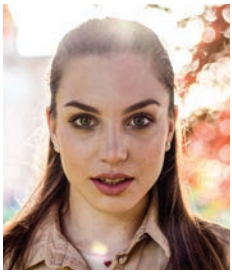
Name: TODA IGNJATOVIĆ

Title: Bachelor Student, III Year

Institution: University of Banja Luka, Faculty of Natural Science and Mathematics

Position: Student

E-mail: toda.ignjatovic@student.pmf.unibl.org



Name: KRISTINA BRATIĆ

Title: Bachelor Student, III Year

Institution: University of Banja Luka, Faculty of Natural Science and Mathematics

Position: Student

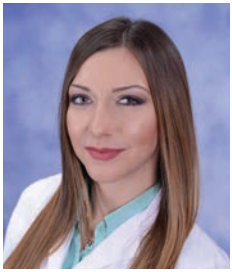
E-mail: kristina.bratic@student.pmf.unibl.org

Antioxidant capacity of *Sorbus torminalis* (L.) Crantz and *Viscum album* L.

Research Field: Plant biochemistry

Abstract: The aim of our work was to examine the content of total phenolic compounds (TPC) and flavonoids in the leaves of *Sorbus torminalis* (L.) Crantz and the leaves and shoots of *Viscum album* L. hosted by *Crataegus monogyna* Jacq. In addition, the goal was to determine the antioxidant capacity using different *in vitro* methods. The obtained results showed that the content of TPC decreases in the order: *V. album* (shoots 16.325 ± 1.556 mg/g) >*V. album* (leaves 11.648 ± 1.267 mg/g) >*S. torminalis* (11.520 ±0.215 mg/g), while the content of flavonoids decreases in the order: *V. album* (leaves 50.627 ± 2.094 µg/g) >*V. album* (shoots 32.856 ± 1.362 µg/g) >*S. torminalis* (29.793 ± 1.023 µg/g).The ethanol extract of the *V. album* leaves showed the highest ability to remove ABTS (2,2'-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid) radicals and hydrogen peroxide, while the extract of *V. album* shoots showed the highest ability to chelate Fe. On the other hand, *S. torminalis* leaves extract had the highest ability to remove DPPH (2,2-diphenyl-1-picrylhydrazyl) radicals. The results indicate that individual phenolic compounds in the extract could have a greater effect on the antioxidant capacity than the total content of phenolic compounds.

Keywords: phenolic compounds, ABTS, DPPH, H_2O_2 scavenging, Fe chelation ability



Name: OLGA GIGOPULU

Title: PhD student

Institution: Faculty of Pharmacy, Ss. Cyril and Methodius University, Skopje

Position: Teaching assistant

E-mail: olga.gigopulu@ff.ukm.edu.mk

Comparison of vibrational spectroscopic techniques for determination of phytocannabinoid content in medicinal *Cannabis sativa* flowers

Research Field: Vibrational spectroscopy, PAT, chromatography, natural products

Abstract: The demand for efficient large-scale cultivation and production of medicinal cannabis has expanded due to the exponential growth of its use for therapeutic purposes. The variability of phytocannabinoid concentrations in plant material, relays greatly on the cultivation practices and for this reason, quality parameters need to be continuously monitored throughout the production process. Over the past few decades, rapidly evolving technology has led to a significant increase in the use of vibrational spectroscopic techniques such as Raman, mid-infrared (MIR), and near-infrared (NIR) spectroscopy combined with chemometric analysis, as powerful methods for industrial research, process monitoring and quality control. Therefore, our main objective was to employ these techniques and to compare them for quantitative analysis of total THC and CBD in medicinal cannabis flowers, aiming to be further utilized as process analytical technology (PAT) in cannabis production. Thus, vast sets of MIR, NIR and Raman spectra of dried cannabis flowers were recorded accompanied with HPLC results for the content of total THC (THC% + 0.877*THCA%) and total CBD (CBD% + 0.877*CBDA%). The collected spectra were subjected to partial least-squares (PLS) analysis to develop calibration models for the quantification of THC and CBD in cannabis flowers. The obtained results indicate that vibrational spectroscopic techniques should be considered as a promising PAT tool for quantification of THC and CBD in medicinal cannabis industry.

Keywords: Raman, MIR, NIR, spectroscopy, hemp, HPLC

Name: DEHUA YANG

Title: Professor

Institution: Shanghai Institute of Materia Medica, Chinese Academy of Sciences

Position: Principal Investigator

E-mail: dhyang@simm.ac.cn

The Chinese National Compound Library – An open innovation platform

Research Field: Receptor Pharmacology

Abstract: The Chinese National Compound Library (CNCL), located at the Pharma Valley of China – Shanghai Zhangjiang High-tech Park, is a major research and development establishment managed by the National Center for Drug Screening, Shanghai Institute of Materia Medica, Chinese Academy of Sciences and Shanghai Zhangjiang Biopharmaceutical Base Development, Co., Ltd. Its storage capacity reached 2.35 million compounds possessing diversified structures up to now. Coupled with this library will be advanced sample handling, information management and quality control systems. CNCL is devoted to the exploration of compound resources within China in order to increase both the size and the structural diversity of the library. This will help to meet the needs of high-throughput screening. The CNCL wishes to collect and optimize chemically diversified compounds and/or natural products from domestic or international sources. As an important material and information resource, CNCL work with both domestic and international stakeholders to promote sustained development of Chinese pharmaceutical industry.

Keywords: Compound library, High-throughput screening, drug discovery

Short biography: Dehua YANG obtained his Ph.D. degree from Shanghai Institutes for Biological Sciences, Chinese Academy of Sciences in 2009 followed by postdoctoral training at Ruijin Hospital, Shanghai Jiao Tong University School of Medicine. After joining Shanghai Institute of Materia Medica, Chinese Academy of Sciences in 2012 as an associate professor, his work has mainly been directed towards structure and functional studies on class B G protein-coupled receptors, namely glucagon receptor, glucagon-like peptide-1 receptors and glucose-dependent insulinotropic polypeptide receptor. He participated in the determination of the 3-D structures and conformational states of these receptors, elucidation of their molecular mechanism for ligand-receptor selectivity, as well as the screening and development of novel ligands targeting G protein-coupled receptors. He was promoted to full professor in 2017.

Name: MIN HE

Title: Director of Graduate Education Office

Institution: Shanghai Institute of Material Medica, Chinese Academy of Sciences

Position: Director of Graduate Education Office

E-mail: hemin@simm.ac.cn

Introduction to international graduate education of SIMM

Research Field: Graduate Education

Abstract: As one of the research units of Chinese Academy of Sciences (CAS), Shanghai Institute of Materia Medica (SIMM) is the only comprehensive institute that dedicated to drug discovery and development. In the meanwhile, SIMM is also an enrollment unit of University of Chinese Academy of Sciences (UCAS) which shoulders the main responsibilities of graduate education with abundant resources, including tutors and experimental facilities. Based on CAS and UCAS, SIMM began to enroll international students in 2013. Up to now, SIMM recruited more than 60 international students, from 19 countries and regions all over the world. With a strong faculty team and advanced research equipment, SIMM has been devoted in international education program to prove its global influence. Besides, with the financial support of UCAS and Chinese government, there exists a series of scholarships for international students. All these mentioned factors will be illustrated with details in this report to make a thorough introduction to the international graduate education program of SIMM.

Keywords: International Education, Faculty, Admission, Scholarship

Short biography:

Education background

- 2006/09–2009/07 PhD., Shanghai Institute of Materia Medica, Chinese Academy of Science
- 2001/09–2004/07 Master, Nantong Medical College
- 1994/09–1999/07 Bachelor, Nantong Medical College

Work Experience

- 2013/11–Present Director of Graduate Education Office. Shanghai Institute of Materia Medica, Chinese Academy of Sciences
- 2011/11–2013/10 Associate professor. The National Center for Drug Screening, Shanghai Institute of Materia Medica, Chinese Academy of Sciences
- 2009/09–2011/10 Research associate. The National Center for Drug Screening, Shanghai Institute of Materia Medica, Chinese Academy of Sciences

Responsibilities

- Graduate students recruitment and training
- Education project and funds management
- Discipline construction and evaluation
- Office strategic planning
- Strategic plan for graduate education development

Name: Viktor Nedović

Title: Full Professor

Institution: Ministry of Science, Technological Development and Innovation (NITRA)

Position: Director of Serbia Accelerating Innovation and Entrepreneurship (SAIGE) Project

E-mail: viktor.nedovic@nitra.gov.rs, vnedovic@agrif.bg.ac.rs

Transformation of R&D landscape in Serbia

Research Field: Biotechnology, Food Technology

Abstract: Serbia Accelerating Innovation and Entrepreneurship (SAIGE) Project supports reform of the science and research sector, strengthening cooperation between the economy and academia, and the development of innovative companies.

Project has three components:

- Component 1 – Research Sector Reforms
  - 1.1 – Serbia Science Fund
  - 1.2 – RDI Reforms
  - 1.3 – Serbian Diaspora Facility
- Component 2 – Enterprise Acceleration (IF)
- Component 3 – Project Implementation, Monitoring, Capacity Building (NITRA)

Ministry of Science, Technological Development and Innovation (NITRA)/SAIGE PIU is responsible for the overall project implementation and monitoring and in particular for support to RDI reforms.

18 RDIs started the transformation process. Project provided financial and technical support for RDIs' institutional reforms and development (capacity building, technology transfer and equipment). Services developed so far: International Advisory Boards, International and National Institutional Consultants, tech transfer capacity building, IP legal support, data management and open access policy improvement, strategy advisory services, Horizon Europe, other competitive programs and project cycle management, environmental, social and ethical issues, HR capacity building, website redesign and digital communications.

Project is supported by the Government of Republic of Serbia, World Bank and European Commission.

Keywords: RDI institutional reform, transformation, capacity building

Short biography: Working activity: Full professor of University of Belgrade; Head of the analytical laboratory and brewing plant pilot at the Faculty of Agriculture; Director of Serbia Accelerating Innovation and Growth Entrepreneurship (SAIGE) project – Ministry of Science, Technological

Development and Innovation. More than ten years served as Assistant Minister and State Secretary in the Ministry responsible for science in Serbian Government.

Research work: Bioencapsulation, fermentation processes (beer fermentation), bioreactor design.

Bibliography: Over 400 articles, more than 100 papers in SCI journals and more than 30 book chapters. He edited five books for the renowned scientific publishers (Kluwer, Springer, CRC Press).

Pedagogical work: Mentor over 40 diploma works, more than 20 master thesis and 5 doctoral theses.

Additionally: Member of the Academy of Engineering Sciences of Serbia (AESS); Coordinator or participant in more than 50 research projects; President of the Serbian Association of Food Technologists (SAFT); President of CEFood 2012 Congress; Chairperson of EFFoST Task Team CEFood congresses; Organizer of national student's competition in the creation of eco-innovative food products, EcoTrophelia Serbia; Co-coordinator of Priority Area Knowledge Society of the EUSDR; Coordinator of Smart Specialization Strategy of Republic of Serbia.

Republic of Serbia

MINISTRY OF SCIENCE,
TECHNOLOGICAL DEVELOPMENT
AND INNOVATION