Scientific Tracks & Abstracts

35 YEARS
OF EXCELLENCE
IN MEDICAL
PUBLISHING

Plenary Session

Session Introduction

Title: SAMET: A machine- learning web based platform for management, interpretation and analysis of IR spectral data

Amirhossein Sakhteman | Shiraz University of Medical Sciences | Iran

Title: Piperine alkaloids and derivatives: Multistage extraction, structural optimization, DFT analysis, and biomedical application

Xin Li | DWI-Leibniz-Institute for Interactive Materials | Germany

Title: Using the 3D printer as a tool for storing, packaging and developing of low cost scientific devices

Ana Luisa Silva | Rio de Janeiro State University | Brazil

Title: Efficacy Medical Countermeasure agent and Chemical therapeutic development for repurposing against Chemical and Biological threat agents, and bio-modelling capabilities of the MCMs for CBRNe agents

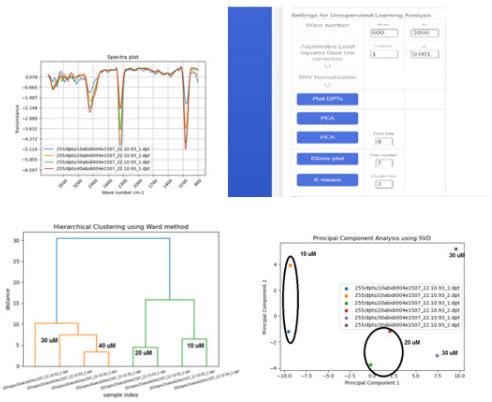
Salako Olatunji | CCACBWA LAGOS | Nigeria

3rd Global Experts Meeting on
Chemistry and Medicinal Chemistry
November 23, 2021 | Webinar

SAMET: A machine- learning web based platform for management, interpretation and analysis of IR spectral data

Amirhossein Sakhteman, Maryam Kabiri
Shiraz University of Medical Sciences, Shiraz, Iran

Versatile supervised and unsupervised machine learning techniques are widely used in different branches of pharmaceutical sciences. Application of supervised techniques including hierarchical cluster analysis (HCA), k-means and kohonen neural network in clustering of different spectral data such as infra-red (IR) spectroscopy can lead to better interpretation as well as investigation of batch to batch variations in chemicals (1). To integrate different unsupervised learning methods as well as providing a suitable management platform in an easy to use interface, we designed and developed a web based software in django frame work by means of python and JS programming (2). SAMET (Spectral Analysis via Machine Learning Estimation of Trained models) can be hosted in both windows and linux operating systems for management and analysis of IR spectral data. This software can visualize, present descriptive interpretation for IR spectroscopy and perform unsupervised learning methods on dpt files resulting from IR spectroscopy. This platform can be utilized in different branches of pharmaceutical industry such as quality control labs.



Biography

Dr. Maryam Kabiri is a PharmD,MPH student with experience in molecular modeling,computational drug discovery, toxicological screening of synthetic and natural products and bioinformatics.The most prominent goal of her research is to find out novel in silico pipelines in drug design and discovery,molecular dynamics simulation of membrane proteins and drug delivery

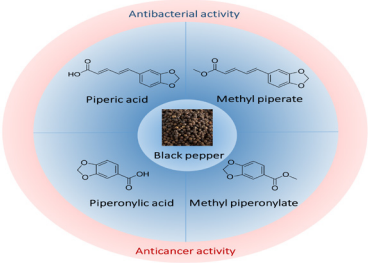
kabiriyasaman8@gmail.com

3rd Global Experts Meeting on
Chemistry and Medicinal Chemistry
November 23, 2021 | Webinar

Piperine alkaloids and derivatives: Multistage extraction, structural optimization, DFT analysis, and biomedical application

Xin Li
DWI-Leibniz-Institute for Interactive Materials, Germany

The natural product, black pepper, plays important roles in the food and pharmaceutical industries since it is rich in versatile bioactive molecules. To achieve the most medicinal value of piperine alkaloids from black pepper, we developed a variety of green and multistage extraction strategies. Encouragingly, these strategies display high extraction yields and purity for the refinement and separation of piperine alkaloids. Furthermore, four bioactive derivatives of piperine alkaloids (i.e., piperic acid, methyl piperate, piperonylic acid, and methyl piperonylate) were prepared through structural optimization. Among them, the formed piperic acid and piperonylic acid with ionizable carboxyl group are able to address the delivery barriers after intravenous injection, due to the improved aqueous solubility. The formed methyl piperate and methyl piperonylate show high membrane permeability for efficient oral absorption. The piperine alkaloids and their derivatives were characterized by 1H and 13C NMR, FTIR, UV-vis and fluorescence spectroscopy, as well as high-performance liquid chromatography (HPLC). Moreover, the density functional theory (DFT) was employed to explore the relationship of geometry structure, energy gap, thermodynamic equilibrium, electronic property, and bioactivity of the piperine alkaloids and derivatives. For biomedical applications, the antibacterial and anticancer activities of piperine alkaloids and derivatives were evaluated and compared. The piperine alkaloids and methyl piperate exhibited the potent antibacterial effect against some types of microorganisms such as S. aureus, S. pyogenes, E. coli, and S. typhi with the lowest MIC of 400 kg/ml, suggesting that piperine alkaloids and methyl piperate can be developed as the excellent antibacterial agents. Likewise, the anticancer effects of piperine alkaloids and derivatives were investigated on different cancer cell lines (e.g., B16, PANC, 4T1, and HeLa cells) using CCK-8 assay. The results revealed that piperine alkaloids possess the best anticancer activity (IC50 = 18.4 kg/mL) for 4T1 cells compared to other derivatives. In summary, our work provided a blueprint for the development and optimization of the next generation of highly effective phytomedicine.



Biography

Xin Li received his M.Sc. degree in Biochemical Engineering from Donghua University in 2017, and Ph.D. degree in Chemistry from RWTH Aachen University in 2021. Then he work as postdoctoral Research Fellow in DWI-Leibniz-Institute for Interactive Materials e.V. He has published more than 50 peer-reviewed SCI-indexed journal articles. His current research interests are focused on the development of phytomedicine, nanoprodrug, intelligent nanocarriers, organic/inorganic hybrid nanoplatforms for biomedical applications, in particular for precision cancer imaging and therapy.

xli@dwi.rwth-aachen.de

3rd Global Experts Meeting on
Chemistry and Medicinal Chemistry
November 23, 2021 | Webinar

Using the 3D printer as a tool for storing, packaging and developing of low cost scientific devices

Ana Luisa Silva
Rio de Janeiro State University, Brazil

Statement of the Problem: The Heritage of Science and Technology consists of instruments and devices, produced and used in scientific research and technological development activities, since they are essential to the process of generating and constructing knowledge. Their presence can be observed in different spaces such as laboratories, universities and research centers. Additionally, they can also be found in museums, science centers and even in private collections reflecting the history and growth of different fields of knowledge. Beyond the functionalities they perform in everyday scientific practice, they can also be used as sources for studies in the field of History of Science and Technology, as complementary educational practices, in research and scientific dissemination activities, for preservation of scientific memory, among multiple other uses. Methodology & Theoretical Orientation: A customized case for the protection of a reference electrode Ag/AgCl was developed and modeled according to the steps of Figure 1 using TinkerCad software for design and Slic3r for slicing and conversion into G-code format. The protection and packaging casing was printed with polylactic acid filament - PLA. Findings: 3D printing has been used for the development of new scientific devices, as identified by Silva et al (2021) in an article on electrochemical cells, in the creation of replicas and mtodels of instruments for exhibition in museums, teaching and research, and in the creation of customized casings for safekeeping and storage of sensitive instruments, as shown in Figure 2. Conclusion & Significance: The use of 3D printing guarantees the preservation and creation of scientific instruments and devices by producing complex shapes with precision and customization according to the dimensions and characteristics of each object, preventing potential risks of damage and degradation that compromise its integrity and usability.

Figure 1. Flowchart of the main stages of the 3D printing process. (Source: Silva et al., 2021)

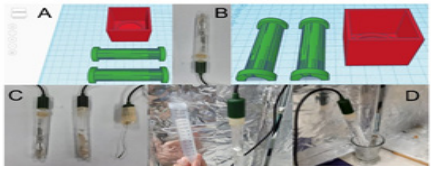


Figure 2. Casing model for a reference electrode protection (A) TinkerCad design (B) Reference electrode in good conditions (C) Damage caused by poor storage (D) Previous improvised storage.

Biography

Currently a Master's student in the preservation of science and technology collections at the Museum of Astronomy and Related Sciences (MAST) and in the preservation of cultural heritage by the National Historical and Artistic Heritage Institute (IPHAN). Graduated in Archival Science by the Fluminense Federal University (2018). Expert in digital preservation, personal archives and heritage conservation. Also works in product development, training and consulting in 3D printing.

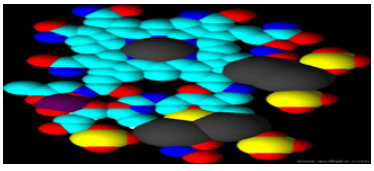
analuisa_als21@hotmail.com

3rd Global Experts Meeting on
Chemistry and Medicinal Chemistry
November 23, 2021 | Webinar

Efficacy Medical Countermeasure agent and Chemical therapeutic development for repurposing against Chemical and Biological threat agents, and bio-modelling capabilities of the MCMs for CBRNe agents

Salako Olatunji
CCACBWA LAGOS, Nigeria

SodaSulphanecobalamin (Na4S5 CoC69N15H89O26) is an effective Medical Countermeasure agent against Chemical and Biological warfare Agents for critical treatment of their acute health effects, which detoxify and decentralized the toxic substances in some chemical based threat mainly. Classical chemical agent threat categories include vesicant or blister agents (e.g., sulfur mustard), blood agents (e.g., cyanide), respiratory agents (e.g., phosgene), and nerve agents (e.g., GA or Tabun, GB or Sarin, GD or Soman, and VX) as well as lung damaging agents (Chlorine, diphosgene). It dissociates the toxic components in each chemical weapon, either nerves agent, blister agent or mustard gas to a nontoxic substance when administered and doesn't have any adverse effects unlike Atropine (which has little effect on nicotinic effect, such as muscle twitching, flaccidity) and other antidotes been tested for neutralizing or countermeasures for a particular chemical-based threat. It displaces the Cyanides to a free toxic compound, thiocyanocobalamin. It removes the burns when the sulfur mustard is been contacted through skin, and eye. The antidote (SodaSulphanecobalamin) which is sulfur drug group (H-S) bends the mustard makes the MCMs removes bumps from the body, which can be used as treatment for Organic Arsenical. It also adds enzyme protease to the body which aid the development of protein in the body. However, recent studies shows that this antidote can serve as a replacement for the antidote of orange agent (2, 3, 4, 7-tetra chlorobenzodioxin) which displaced millions of Vietnam Citizens during the World War II and removes completely the w chlorine atoms attach to the benzene ring to sodium benzoate and saline. Though Mercury (I) Oxalate is been used for this antidote for the orange agent, but we all know that Mercury is highly toxic and poisonous to the human. When SodaSulphanecobalamin is been used for nerves MCMs agents, it dissociates organophosphate to phosphonic acid which helps in metabolism of the body. Baseline mean weights, time to hypotension (31 minutes 3 seconds versus 28 minutes 6 seconds), and the chemical threat agents' dose at hypotension (5.6 versus 5.9 mg/kg) were similar. One animal in the SodaSulphanecobalamin group and 2 animals in the sodium nitrite group died during antidote infusion and were excluded from analysis. SodaSulphanecobalamin resulted in a faster return to baseline mean arterial pressure, with improvement beginning at 5 minutes and lasting through the conclusion of the study (P<.05). No statistically significant difference was detected between groups for cardiac output, pulse rate, systemic vascular resistance, or mortality at 40 minutes post intoxication.



Biography

Xin Li received his M.Sc. degree in Biochemical Engineering from Donghua University in 2017, and Ph.D. degree in Chemistry from RWTH Aachen University in 2021. Then he work as postdoctoral Research Fellow in DWI-Leibniz-Institute for Interactive Materials e.V. He has published more than 50 peer-reviewed SCI-indexed journal articles. His current research interests are focused on the development of phytomedicine, nanoprodrug, intelligent nanocarriers, organic/inorganic hybrid nanoplatforms for biomedical applications, in particular for precision cancer imaging and therapy.

Salakoolatunji9@gmail.com

PULSUS
WWW.PULSUSCONFERENCE.COM

Accepted Abstracts

35 YEARS
OF EXCELLENCE IN MEDICAL PUBLISHING

The support of the E.U. ICARE AMIF Project in the detection of SARS- COV-2, sublineage in migrants arriving to Italy via the Mediterranean Sea and public health implication

Antonio Sparaco
Global Health Center Director, Trapani

With the arrival of Covid-19 epidemic in the regions of southern Italy, the attention on the health of migrants from countries with strong migratory pressure has been amplified more and more.

The interventions for the protection of public health have been reformulated also because the recent scientific evidence on the possible neutralization of the effects of vaccine by the new mutated viral strains are generating further worries among the population.

The establishment of quarantine ships is helping to protect public health more efficaciously, acting as a filter for the resident population and ensuring more rational assistance to migrants arriving in the region.

To safeguard national public health, the Italian Ministry of Health has entrusted the Region Sicily with the implementation of an epidemiological surveillance project of Covid-19 on the region and in other territorial contexts in Italy, to define the impact that the epidemic has on the foreign population.

In this context, the Local Health Department of Trapani collaborates for the management and sharing of oropharyngeal samples used for the search for variants to identify new models of diffusion and reconstruction of samples of migratory flows. Moreover, the project provides of a training intervention aimed at the operators of the health authority. From the beginning of the survey of Covid 19 virus in migrants (November 2020), carried out by our department, there have been more than 5.467 swabs performed on migrants of which 110 were positive.

In this regard, also the E.U. ICARE project continues to give an important support, for the sustainability of the actions both in procedural / instrumental terms and in terms of prevention and health care.

In fact, during scheduled landings, the supply of rapid tests and the rapid execution of it, allows the immediate identification of positive subjects to Covid 19.

On the other hand, when the landings of migrants arriving through the Mediterranean sea occur in a widespread manner and with few migrants, the greatest difficulty is the lack of prompt intervention for the execution of swabs.

3rd Global Experts Meeting on
Chemistry and Medicinal Chemistry
November 23, 2021 | Webinar

Title: Liposomes-based Immunoassay for the Detection of Cardiac Troponin I —A Gold-Standard Biomarker for the Diagnosis of Myocardial Infarction

Remya Radha
American University of Sharjah,, UAE

Cardiovascular diseases (CVDs) are the leading causes of death in intensive care units worldwide, particularly in UAE and Mediterranean countries. The World Health Organization stated that by 2030, almost 23.6 million people will die from CVDs. The buildup of plaque and blockage of arteries leads to potentially deadly acute myocardial infarction (MI), known as "heart attack". Electrocardiography (ECG) is one of the common diagnostic tools for spotting and triaging MI patients however more than 40% of MI cases show normal ECG profile while testing. The measurement of certain biomarkers in the patient blood could provide a more accurate diagnosis of MI. Cardiac troponin I (cTnI), the central key element of cardiac muscle regulation and contraction, is considered the standard biomarker for the diagnosis of MI. This study reports the development of an efficient fluorescent immunoassay for the detection and quantification of cTnI using liposome-based fluorescent signal amplification. The assay is based on capturing cTnI molecule between a surface-immobilized capturing antibody and a biotin-conjugated secondary antibody (detection antibody). Signal dvelopement was achived by subsequent addition steps of streptavidin and biotin-conjugated liposomes which are loaded with a fluorescent dye. The fluorescent signal is greatly enahanced upon the release of loaded dye from the liposomes. The standardized assay is sensitive and selective towards cTnI both in physiological buffer solutions and human serum samples and provides a wide linear dynamic range relvant to clinical concnetrations.

3rd Global Experts Meeting on
Chemistry and Medicinal Chemistry
November 23, 2021 | Webinar

New resources from timber waste: bioactive constituents obtained by "smart chain extraction"

Stefano Dall'Acqua
University of Padova, Italy

Coniferous barks are known for high content in bioactive compounds with potential high bioactivities in several area. Timber industry is producing large amount of bark waste as result of wood cutting and preparation. In this paper an innovative extraction approach based on the sequential application of Supercritical CO2 extraction, microwave or ultrasound assisted extraction with green solvents (water-based mixture with minimum amounts of ethanol) will be applied to Picea abies barks and wood, obtaining extracts enriched in bioactive secondary metabolites. Detailed analysis using LC-DAD-MSn GC-MS, NMR, FT-IR have been performed, and main constituents were identified and quantified on each extract. PiceasideG, piceaside H, taxifolin, taxifolin glucoside, trachelogenin, 7-Hydroxymatairesinol, 7-oxo matairesinol were the most abundant polar secondary metabolites. Volatile constituents extracted with microwave distillator were identified as eucalyptol, □ and β pinene. More lipophylic constituents mostly extracted during the first step in CO2 were dehydroabietic acid, cinnamic ester with fatty acids. Obtained fractions have been subjected to different bioassays related to antioxidant and metal chelating activity (DPPH, ABTS, CUPRAC, FRAP, MCA, PMB). Furthermore, inhibitory assays on enzymatic activities were performed namely acetylcholinesterase, butyrilcholinesterase, tyrosinase, amylase and glucosidase. Some extracts present very high antioxidant activity and significant tyrosinase effect thus being good candidate for topic application as cosmetic or pharmaceutical treatments for skin hyperpigmentation. Other fractions revealed significant inhibitory activity on cholinesterase. Thus, further studies are in progress to assay isolated compounds.

The overall results showed the application of an innovative extractive approach based on green chemistry principles and combining different techniques. Obtained extracts demonstrated the opportunity to exploit timber industry waste as source of bioactive constituents.