

# **CHEMISTRY** in Sri Lanka

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## Chemistry for Quality Life

The Tri Annual Publication of the Institute of Chemistry Ceylon

Successor to the Chemical Society of Ceylon, founded on 25 <sup>th</sup> Jan Vol. 42 No. 2	May 2025
	Pages
Council 2024/2025	02
Dutline of our Institute	02
Guest Editorial	
Prospects of Peptides in Nanotechnology	03
54 <sup>th</sup> Annual Sessions and 84 <sup>th</sup> Anniversary Celebrations 2025	
Inauguration of the 54 <sup>th</sup> Annual Sessions	06
Distinguished Service Award - 2025	07
Special Yeoman Service Award – 2025	10
Long service awards - 2025	11
Chandrasena Memorial Award - 2025	13
Kandiah Memorial Graduateship Award -2025	15
Professor M. U. S. Sultanbawa Award for Research in Chemistry - 2024	17
CCS Researcher of the Year Award - 2025	20
Theme Seminar on Chemistry for Quality Life	21
Technical Sessions Programme	26
Abstracts of Research Papers to be presented at the 54 <sup>th</sup> Annual Sessions 20	32

## Chemistry for Quality Life

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## **Outline of our Institute**

The Institute of Chemistry Ceylon is a professional body and a learned society founded in 1971 and incorporated by act of Parliament No. 15 of 1972. It is the successor to the Chemical Society of Ceylon which was founded in 1941. Over 50 years of existence in Sri Lanka makes it the oldest scientific body in the country.

The Institute has been established for the general advancement of the science and practice of Chemistry and for the enhancement of the status of the profession of Chemistry in Sri Lanka. The Institute represents all branches of the profession and its membership is accepted by the government of Sri Lanka (by establishment circular 234 of 9-3-77) for purposes of recruitment and promotion of chemists.

#### **Corporate Membership**

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## Full membership is referred to as corporate membership and consists of two grades: Fellow (F.I.Chem.C.) and Member (M.I.Chem.C.)

Application for non-corporate membership is entertained for four grades: Associate (former Graduate) (A.I.Chem.C.), Licenciate (L.I.Chem.C.), Technician (Tech.I.Chem.C.) and Affiliate Member.

#### **Revision of Membership Regulation**

All Special Degree Chemists can now apply directly to obtain Associate (Graduate) Membership. Three year B. Sc. Graduates (with an acceptable standard of Chemistry) can

(i) directly become Licentiate

(ii) obtain corporate membership in a lesser number of years.

#### Tech.I.Chem.C.

Those who have passed the DLTC examination or LTCC examination or have obtained equivalent qualification and are engaged in the practice of Chemistry (or chemical sciences) acceptable to the Council are entitled to the designation Tech.I.Chem.C.

Members/Fellows with Membership for Life are entitled to the designation of **Chartered Chemist (C.Chem.)** on establishment of a high level of competence and professionalism in the practice of chemistry and showing their commitment to maintain their expertise.

All corporate members (Members / Fellows) are entitled to vote and become Council/ Committee members whether Chartered Chemists or not.

#### **Membership Applications**

Any application for admission to the appropriate class of membership or for transfer should be made on the prescribed form available from the Institute Office.

#### **Current Subscription Rates**

Fees should be payed on 1st of July every year and will be in respect of the year commencing from  $1^{st}$  July to  $30^{th}$  June

Fellow	Rs. 2000
Member	Rs. 2000
Associate	Rs. 1500
Licenciate	Rs. 1200
Technician	Rs. 750
Affiliate	Rs. 1200
Membership for Life	Rs. 15000

#### **Entrance Fee**

All the grades	Rs. 1000
Processing Fees*	Rs. 500
Processing Fee for	
Chartered Chemist designation	Rs. 5000
Institutional Members	Rs. 2500
*per application for admission/transfer to a	ny grade

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## **Guest Editorial**

## Prospects of Peptides in Nanotechnology

Dr. Laksiri Weerasinghe

Department of Chemistry, Faculty of Applied Sciences, University of Sri Jayewardenepura Email: laksiri@sjp.ac.lk

#### 1.1. Introduction to Peptides

Short sequences of amino acid residues connected by amide linkages are referred to as peptides [1]. Traditionally, peptides with fewer than 20 amino acids are referred to as oligopeptides, and those with between 20 and 100 amino acids are referred to as polypeptides. Structurally peptides are arranged in an array of structural forms including linear, cyclic, and depsipeptides. Modified peptides with various nonpeptide moieties, such as phosphoryl groups or carbohydrates (phosphopeptides or glycopeptides), polyketides, or terpenoids are also found in nature [2].

Besides their unique biological activities, peptides have gained a great deal of interest recently due to their unique features such as biocompatibility, stability, and specificity. With their potential use in biosensing, tissue engineering, and drug delivery, peptide-based nanostructures have gained a great deal of interest recently in the realm of nanotechnology [3]. However, understanding the fundamentals of peptides including the synthesis and characterization is key to the expansion of their application in nanotechnology.

The principles of Peptide Synthesis involve the sequential joining of amino acids to create peptide chains [4]. Primarily peptide synthesis can be done using solid-phase peptide synthesis (SPPS), liquid-phase peptide synthesis, and native chemical ligation. Currently, the most common method is Solid-phase peptide synthesis, or SPPS, in which the process of creating peptides by joining the initial amino acid to a solid support, adding subsequent amino acids one by one, and finally splitting the peptide from the solid support [5]. Protecting groups also play a critical role by ensuring the chemo-selective in peptide synthesis [6].

#### 1.2. Peptides and nanotechnology

Peptides and nanotechnology are two distinct fields that have emerged as crucial tools in the biomedical sciences in recent years. Hence, a basic understanding of each field could be useful for future scientists and science contributors in peptides and nanotechnology.

Peptides have been incorporated into nanotechnology since the early 1990s. The potential of peptides as building blocks for nanostructures was first recognized by Ghadiri and coworkers [7]. Since then, various investigations into the usage of peptides in nanotechnology have been carried out, and many peptide-based nanomaterials have been developed for a wide range of biomedical applications.

Currently, peptide-based nanomaterials are mainly used for drug delivery applications. One of the earliest examples was the development of liposomes decked with cyclic RGD peptides for targeted carriers of anticancer drugs. Another early example was the development of nanoparticles composed of a block copolymer and a peptide that targeted avß3 integrin receptors for imaging and drug delivery applications [8]. Peptide-based nanomaterials have now been created for a variety of applications as the area has rapidly grown, including cancer therapy, tissue engineering, biosensors, and imaging. The development of various peptide-drug conjugates was facilitated through the application of peptides to enhance the stability and solubility of poorly soluble medicines.

The use of peptides in nanotechnology has also been driven by advances in peptide synthesis techniques. SPPS, which was first presented in the 1960s, has revolutionized the field of peptide chemistry and has made it possible to synthesize peptides with a high degree of purity and accuracy. SPPS has also enabled the synthesis of complex peptides, including cyclic peptides and peptide-based macrocycles, which have been appealing for use in nanotechnology applications because of their distinctive qualities.

Peptides have several chemical properties that make them useful in nanotechnology. One of the most important is their ability to form strong, specific interactions with other molecules. This is caused by the presence of functional groups in the peptide chain's amino acid residues. For example, the amino group  $(-NH_2)$  and a carboxyl group (-COOH) on each end of the peptide can form hydrogen bonds with other molecules, allowing peptides to link with specific targets with high affinity and preciseness [9]. Additionally, some amino acids have unique chemical properties. The sulfur-containing amino acid cysteine can form disulfide bonds with other cysteine residues to create stable three-dimensional structures [10].

Peptides also have several physical properties that make them useful in nanotechnology. Their size represents one of their most crucial characteristics. Peptides are typically much smaller than proteins, from a few hundred to several thousand molecular weight Daltons. This small size makes them ideal for use in nanoscale applications, where precise control over size and shape is critical. Another important physical property of peptides is their conformational flexibility. Peptides can adopt a wide range of conformations, including helical, beta-sheet, and random coil structures. This flexibility allows peptides to fold into specific threedimensional shapes and interacts with other molecules in a variety of ways. Finally, peptides have also excellent biocompatibility and biodegradability, which make them ideal for use in biomedical applications. They can be synthesized from natural amino acids or modified amino acids to enhance their properties and can be easily degraded by natural processes in the body [11].

#### 1.3. Prospects of nano-peptides chemistry

The growing interest in creating peptide-based nanomaterials has been observed recently with advanced functionalities such as stimuli-responsive behavior, targeting specificity, and controlled release. The ability to incorporate functional moieties into peptides has opened a new avenue for the development of smart nanomaterials that can respond to various external stimuli such as pH, temperature, and light.

One of the most promising applications of peptides in nanotechnology is in the field of drug delivery. Peptide-based drug delivery systems have the potential to improve the therapeutic index of drugs by enhancing their solubility, stability, and bioavailability. Furthermore, peptide-based systems can target specific cells or tissues, limit the side effects of medication while improve their efficacy.

Peptides also hold great promise in tissue engineering and regenerative medicine. Peptide-based scaffolds can provide a favorable microenvironment for cell growth and tissue regeneration. They can also promote cell adhesion, migration, and differentiation, which are essential for tissue engineering. Another exciting area of research in peptide nanotechnology is the development of peptide-based biosensors. Such biosensors can detect a variety of analytes, such as proteins, nucleic acids, and small molecules, with high specificity and sensitivity. Peptide-based biosensors are suitable for a range of uses, such as disease diagnosis, environmental monitoring, and food safety.

Despite the significant advances made in peptide nanotechnology, several challenges remain. One of the main challenges is the lack of robust and scalable methods for peptide synthesis and characterization.

Furthermore, the development of peptidebased nanomaterials with advanced physicochemical characteristics of peptides is critical to comprehending functions, which can be challenging as well. Peptides have shown as an alternative building blocks of several nanotechnological submissions due to their unique properties. The ability to incorporate functional moieties into peptides has created a new path for the development of smart nanomaterials with advanced functionalities. Peptide-based drug delivery systems, tissue engineering scaffolds, biosensors, and imaging agents are some of the promising applications of peptides in nanotechnology. However, several challenges remain, and further research is required to overcome these challenges and unlock the full potential of peptides in nanotechnology.

#### References

- Gentilucci, L.; De Marco, R.; Cerisoli, L. Chemical modifications designed to improve peptide stability: incorporation of non-natural amino acids, pseudo-peptide bonds, and cyclization. *Current pharmaceutical design* 2010, *16* (28), 3185-3203.
- 2. Jakubke, H.-D.; Sewald, N., Peptides from A to Z: a concise encyclopedia. John Wiley & Sons: 2008.
- Harish, V.; Tewari, D.; Gaur, M.; Yadav, A. B.; Swaroop, S.; Bechelany, M.; Barhoum, A., Review on nanoparticles and nanostructured materials: Bioimaging, biosensing, drug delivery, tissue engineering, antimicrobial, and agro-food applications. *Nanomaterials* 2022, 12 (3), 457.
- Sheppard, R., The fluorenylmethoxycarbonyl group in solid phase synthesis. Journal of peptide science: an official publication of the European Peptide Society 2003, 9 (9), 545-552.
- Amblard, M.; Fehrentz, J.-A.; Martinez, J.; Subra, G., Methods and protocols of modern solid phase peptide synthesis. *Molecular biotechnology* 2006, 33, 239-254.

- Behrendt, R.; White, P.; Offer, J., Advances in Fmoc solid-phase peptide synthesis. *Journal of Peptide Science* 2016, 22 (1), 4-27.
- Ghadiri, M. R.; Granja, J. R.; Milligan, R. A.; McRee, D. E.; Khazanovich, N., Selfassembling organic nanotubes based on a cyclic peptide architecture. *Nature* 1993, *366* (6453), 324-327.
- 8. Visakhapatnam, P., Indian craftsmen, artisans used nanotech 2000 years ago. Deccan Herald 2008, 1.
- Ray, A.; Nordén, B., Peptide nucleic acid (PNA): its medical and biotechnical applications and promise for the future. *The FASEB Journal* 2000, *14* (9), 1041-1060.
- Morgan, R. S.; Tatsch, C. E.; Gushard, R. H.; Mcadon, J. M.; Warme, P. K., Chains of alternating sulfur and Π-bonded atoms in eight small proteins. *International journal of peptide and protein research* 1978, *11* (3), 209-217.
- Ulery, B. D.; Nair, L. S.; Laurencin, C. T., Biomedical applications of biodegradable polymers. Journal of polymer science Part B: *polymer physics* 2011, 49 (12), 832-864



**Dr Laksiri Weerasinghe** is currently serving as a senior lecturer at the Department of Chemistry, University of Sri Jayewardenepura. He obtained his BSc (Honours) degree in Chemistry from the University of Colombo & PhD from Washinton state University, USA. He is a postdoctoral fellow, University of Montreal, Canada, Washington State University, USA and Sri Lanka Institute of Nanotechnology.

## INSTITUTE OF CHEMISTRY CEYLON 54<sup>th</sup> Annual Sessions and 84<sup>th</sup> Anniversary Celebrations 2025

## Inauguration of the 54<sup>th</sup>Annual Sessions, Institute of Chemistry Ceylon

Monday, June 16<sup>th</sup> 2025 at BMICH

### Programme

8.30 am	Arrival of Guests (refreshments will be provided)
9.30 am	Ceremonial Procession of Council Members and Past Presidents
9.40 am	Lighting of the Oil Lamp & National Anthem
9.50 am	Welcome Address & Presidential Address <b>Prof. Janitha A. Liyanage,</b> <i>President, Institute of Chemistry Ceylon</i>
10.30 am	Address by the Chief Guest <b>Prof. Saranjit Singh</b> <i>Vice Chancellor, Kalinga Institute of Industrial Technology (KIIT), Odisha, India</i>
10.50 am	<ul> <li>Presentation of Awards, Prizes and Certificates</li> <li>Institute of Chemistry Ceylon Awards</li> <li>Distinguished Service Award</li> <li>Yeoman Service Award (Special)</li> <li>Long Service Awards</li> <li>Chandrasena Memorial Award</li> <li>Kandiah Memorial Graduateship Award</li> <li>Professor M U S Sultanbawa Award for Research in Chemistry – 2024</li> </ul>
11.20 am	Address by the Guest of Honour <b>Prof. Uday Maitra</b> <i>President, The Chemical Research Society of India (CRSI)</i>
11.30 am	<ul> <li>Presentation of Awards, Prizes and Certificates</li> <li>CCS Research Awards</li> <li>All Island Interschool Chemistry Quiz prizes</li> <li>National Chemistry Olympiad prizes</li> <li>Graduateship in Chemistry &amp; BSc Hons (Chemical Science) Examinations Scholarships, Prizes and Awards J N Oleap Fernando Memorial Scholarship</li> <li>CCS Awards - Colours</li> <li>Awards for Activities</li> </ul>
12.15 pm	Chandrasena Memorial Award Lecture Prof. A. P. Attanayake
12.35 pm	Vote of Thanks <b>Prof. Hema Pathirana,</b> <i>President Elect, Institute of Chemistry Ceylon</i>

12.40 pm Close of Ceremony

## Distinguished Service Award – 2025 Professor Sudantha Liyanage



Sudantha Liyanage, a product of Thurstan College, Colombo commenced his profession in the field of education way back in 1991 when he joined the University of Sri Jayewardenepura, his alma mater, as an assistant lecturer. He obtained his Ph.D. on a Commonwealth scholarship from the University of Cardiff, Wales, UK in 1996 and returned to Sri Lanka immediately afterwards to commence work as a senior lecturer at the University of Sri Jayewardenepura in 1997. He is a dynamic person, a man of vision and wisdom. Academically, he climbed every rung of promotion ladder, up to Senior Professor in 2017. Simultaneously, he advanced in administration, becoming the first alumnus Dean in the Faculty of Applied Sciences in 2010, a post that he held for 09 consecutive years, longest such tenure in the university system in Sri Lanka, then Dean of the Faculty of Technology in 2019 and eventually becoming the Vice-chancellor, the pinnacle of his career, in 2020. Snr. Prof. Sudantha Liyanage, was instrumental in building a strong and self-sustained faculty-university. During his tenure there was a notable increase in the number of both students and correspondingly academic staff. Self-less man, he motivated and mentored academics to achieve their professional and personal goals. He was a role model for students; nurturing, inspiring and empowering them to become global citizens. Many faculties benefited the state-of-the-art infrastructural developments to support learning and teaching under his leadership. Despite heavy administrative duties, Snr. Prof. Sudantha Liyanage was at the forefront of teaching and research. He has many publications to his credit. Books authored by him are used even today by undergraduates and G.C.E. A/L chemistry students. Presidential Award

for Research in 2019/20 is one of many accolades he has received for scientific contribution and research.

Snr. Prof. Sudantha Liyanage's unwavering commitment to the progress of the University of Sri Jayewardenepura is commendable. Today, the University of Sri Jayewardenepura has achieved the position of the secondbest university in Sri Lanka in the QS World University Rankings 2025. He had equivalent commitment to serve the Institute of Chemistry Ceylon utilising his knowledge, skills and years of experience in the education field.

Institute of Chemistry Ceylon is the only professional body for the general advancement of Chemical Sciences and the practice of Chemistry in Sri Lanka. Snr. Prof. Sudantha Liyanage has contributed immensely to the progress of the Institute of Chemistry Ceylon. He is a Fellow and a Chartered Chemist and has served the Council of the Institute of Chemistry Ceylon as a member since 2002 and the key positions held by him in the Council during this time are as follows;

- Chairman, College of Past Presidents', Institute of Chemistry Ceylon (2021-to date)
- President, Institute of Chemistry, Ceylon (2018-2019)
- President Elect, Institute of Chemistry, Ceylon (2017-2018)
- Vice President, Institute of Chemistry Ceylon (2016-2017)
- Member, Academic Board, Institute of Chemistry Ceylon (2002- to date)
- Member, Board of Examiners, Institute of Chemistry Ceylon (1998- 2022)
- Hon. Editor, Institute of Chemistry Ceylon (2003-2004 and 2008-2009)
- Chairman, Building Committee (2021- to date)
- Chairman, Inter-School Quiz Committee, Institute of Chemistry Ceylon (2002-2003)
- Member, Social Committee, Institute of Chemistry Ceylon (2002-2004)
- Member, Admissions and Ethical Practices Committee (2019-2023) and

#### The Tri-Annual Publication of the Institute of Chemistry Ceylon

• Chairman, Building Committee (2019 – to date).

Furthermore, Snr. Prof. Sudantha Liyanage has contributed immensely to the upliftment of the educational programmes and activities conducted by the College of Chemical Sciences and has served as a visiting lecturer and examiner of the Graduateship in Chemistry programme from 1998 to 2020. He was a pioneering member to initiate the existing B.Sc. Programme in Chemical Science and the Malabe building project. He was also the Chairman of the Royal Society of Chemistry (Sri Lanka Section) from 2006 to 2008 and 2013 to 2014 and the Secretary from 2002-2004.

In addition, Snr. Prof. Sudantha Liyanage served the nation by holding key positions in the following;

- Governing Council, Tertiary and Vocational Education Commission, Sri Lanka (2019 - 2024)
- Governing Council, Association of Commonwealth Universities (2022 2024)
- Standing Committee for Quality Assurance and Accreditation, Ministry of Higher Education, Sri Lanka (2015-2023)
- Presidential Task Force for Education (2020-2022)
- Select Committee of Parliament: Electoral Reforms

(2003-2009 and 2021-2023)

- Academic Board, National Institute of Education (2020-2023)
- Academic Council, National Institute of Business Management, Sri Lanka (2016-2022)
- University Grants Commission, Sri Lanka (2014-2015)
- Director Board, Industrial Technology Institute (2013-2015) and
- Chairman of the Sri Lanka Rupavahini Corporation (June – September 2024).

Over the past few years, he has led the team in completing the magnificent Malabe IChem Building. In addition, throughout the years, Prof. Liyanage has played a significant and valuable role in the development of the Institute of Chemistry Ceylon. In recognition of the valuable and dedicated service rendered by him on behalf of the Institute, the Council of the Institute of Chemistry Ceylon has unanimously decided to award Professor Sudantha Liayanage the Distinguished Service Award at the 54<sup>th</sup> Annual Sessions of the Institute of Chemistry Ceylon in 2025.

## **Cover Page**

This year's presidential theme, "Chemistry for Quality Life," celebrates the transformative role of chemistry in addressing global challenges and enhancing everyday living.

This vibrant illustration captures how chemistry enriches everyday life. At the core is a laboratory flask, symbolizing innovation, surrounded by icons representing health, sustainability, nutrition, clean energy, and medicine. Together, they reflect the essential role chemistry plays in advancing human well-being, environmental protection, and a healthier future.

Chemistry is at the heart of innovations that make life healthier, safer, and more sustainable. From clean water and renewable energy to modern medicine and nutritious food, chemistry empowers solutions that improve the quality of life. This illustration symbolizes how science connects with everyday essentials — shaping a better world through the power of molecules.

To celebrate this important theme, the Institute of Chemistry has organized a seminar featuring four distinguished foreign resource persons who will share their insights and expertise on this vital topic.

(see pages 20-25)

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## Distinguished Service Award – 2025 Mr. N M S Hettigedara



Mr. N. M. S. Hettigedara is an exceptional figure in Sri Lanka's scientific, public, and clinical health landscape, whose expansive career spans over three decades. His journey is marked by distinguished service in chemistry, pharmacy, nutrition, and public health. He is a Chartered Chemist, Registered Dietitian Nutritionist, Registered Pharmacist, and a Fellow of both the Institute of Chemistry Ceylon (IChemC) and the Dietitians' Association of Sri Lanka (DIASL). From 2001 to 2024, he served as Superintendent of Police and Senior Nutritionist at the Sri Lanka Police Hospital. He also functions as a consultant for national-level nutrition and public health initiatives, currently serving the Army Hospital in Colombo and regularly visiting the Cardiac Rehabilitation Programme at the Institute of Cardiology, National Hospital of Sri Lanka. He has also been a former member of the Food Advisory Committee of the Ministry of Health and serves as an expert committee member of the Ministry of Trade.

Mr. Hettigedara's academic journey includes a Graduateship in Chemistry from IChemC (1991), a Bachelor of Pharmacy (Hons) from the Open University of Sri Lanka (2019), and a Master of Science in Food Science & Nutrition from the University of Kelaniya (1995). He is presently pursuing his PhD. His strong academic foundation and commitment to evidencebased healthcare led him to roles as a community pharmacist, pharmaceutical manager, and senior public health officer. His multidisciplinary expertise has been a driving force in improving clinical nutrition practices and pharmaceutical governance in Sri Lanka.

At the Institute of Chemistry Ceylon, Mr. Hettigedara's active involvement began in 1992 and has remained

consistent and impactful. He has served in numerous key leadership positions including President (2022– 2023), Vice President (2020–2021), Secretary (2004– 2008), Treasurer (2008–2012), and Assistant Treasurer (2015–2016). Since 2000, he has been a dedicated Council Member and has contributed significantly to the Institute's academic and policy functions. His committee work spans the Academic Board (1993–2014, 2016/17), Awards Committee, House and Finance, Training and Seminars, Social Affairs, and the Monograph Committee. He was also Chairman of the Professional Recognition Committee (2014–2020) and contributed to the launch of the Diploma in Laboratory Technology and other academic reforms that have elevated the Institute's national reputation.

His national-level coordination of the International Year of Chemistry (IYC) 2011 in Sri Lanka as Chairman of the Organizing Committee was a landmark achievement. Under his guidance, IChemC launched impactful public education initiatives, including the national CHEMEX exhibition and Sri Lanka's first-ever National Titration Competition. These activities significantly enhanced public appreciation for chemistry's role in national development, education, and sustainable practices.

In recognition of his exemplary service to the field of chemistry, Mr. Hettigedara was awarded the prestigious Institute of Chemistry Ceylon Gold Medal in 2012 becoming the first recipient under a newly established criteria framework. His contributions were again recognized with the Distinguished Service Award in 2025, honoring over three decades of leadership, mentorship, and advocacy that have strengthened the Institute's academic standing and national influence.

His impact is equally notable in the Dietitians' Association of Sri Lanka, where he served as Acting President (2014– 2015) and President (2015–2021). Under his leadership, the Association advocated for the formal recognition of dietitians as essential health professionals under the Sri Lanka Medical Ordinance, enhanced ethical regulations, and advanced academic training and practice standards for dietitians and nutritionists across the country.

Beyond institutional leadership, he has served as a

consultant nutritionist to the Sri Lanka Army Medical Services since 1998 and has been a founding member of the Cardiac Rehabilitation Programme at the National Hospital of Sri Lanka since 2002. He has also contributed to national health policies, academic training programs, and public health media campaigns through platforms such as Manusath Derana and TNL's 'Waidya Hamuwa.' Mr. Hettigedara's philosophy is grounded in the belief that science must serve society. His vision aligns closely with the United Nations Sustainable Development Goals (SDGs), emphasizing scientific leadership, evidencebased nutrition, and ethical public service. Through his enduring work across chemistry, pharmacy, and dietetics, Mr. Hettigedara continues to inspire excellence, innovation, and integrity throughout Sri Lanka's health and scientific communities.

## Yeoman Service Award (Special) – 2025 Professor Ramanee D Wijesekera



It is with great respect and gratitude that we recognize **Professor Ramanee D. Wijesekera** for her exemplary service to the Institute of Chemistry Ceylon over the past 25 years. Her unwavering commitment has been evident through her extensive involvement in numerous committees and leadership roles. She has served on the Council since 2005, Hony. Joint Secretary, Institute of Chemistry Ceylon (2009/2010) and as the Dean of the College of Chemical Sciences (2021/2022).

She has also significantly contributed to finance, student affairs, international relations, publications, and editorial work, which is evident from her services to many committees in various capacities as detailed below. Chairperson Awards Committee (2023/2024 and 2018/2019); Chairperson, Awards Committee (2023/2024 & 2018/2019); Member, Awards Committee (2024/2025, 2020 -2023, 2011/2012 and 2009/2010); Chairperson, Academic Board, of the Institute of Chemistry (2021/2022); Member, Academic Board of the College of Chemical Sciences (2019/2020, 2018/2019, 2017/2018, 2016/2017, 2015/2016, 2014/2015, 2011/2012 & 2009/2010); Coopted member (2012/2013 &

2013/2014); Member, Monograph Committee (2006 to date??); Chairperson, Library Committee (2024/2025); Secretary, International Relations (2012 -2018, and 2023 to date); Chairperson, Academic Board Finance, (2021/2022); Chairperson, Student Finance Management Committee (2021/2022); Member, Salary & Cadre Committee (2021/2022); Member, Building Committee (2021/2022); Member, Social Affairs Committee (2018/2019, 2017/2018); Member, Editorial & Publicity Committee (2017/2018, 2016/2017, 2009/2010, 2008/2009); Secretary, House, Finance & Membership Committee (2009/2010); Member, Training Seminars/ Workshops Committee (2009/2010); Hony. Assistant Editor (2007/2008); Editor, Book of Abstracts, Chemtech 2007 International Conference (ISSN 1800-2994); Editor, Proceedings of Chemtech 2007 International Conference (ISSN 1800-3745) are the committees Prof. Wijesekera served over the past 25 years.

Beyond her service to the Institute, Professor Wijesekera concluded a distinguished academic career as a Senior Professor at the Department of Chemistry, University of Colombo, retiring in 2024 after 40 years of service. Her tireless contributions have left an indelible mark on both the Institute and the broader chemical sciences community.

## Long Service Awards - 2025

### Mrs. H. L. Anoma Champanie



The Institute of Chemistry Ceylon is proud to present the Long Service Award to **Mrs. H. L. Anoma Champanie** in recognition and appreciation of her 35 years of uninterrupted, dedicated, and loyal service to the Institute.

Mrs. Anoma Champanie joined the Institute in 1990 as a Trainee Accounts Clerk. Her dedication and commitment led to her promotion as Senior Accounts Assistant in 1998. In 2008, she assumed duties as Assistant Accounting Officer, and in 2013, she was promoted to Senior Accounting Officer. Since January 2020, she has served with distinction as the Assistant Finance Manager.

We extend our sincere gratitude for her invaluable contributions and dedicated service over the past three decades.

## Mr U. J. Nishan Chandana



**Mr U. J. Nishan Chandana** joined the Institute of Chemistry Ceylon in 1999 as a Peon. In 2016, Mr. Nishan was appointed as an Office Assistant, in which he continues his duties with diligence and discipline to this date.

In appreciation of over 25 years of devoted service to the Institute of Chemistry Ceylon, Mr Nishan Chandana is awarded with the Long Service Award.



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Mr H. L. R. H. Abeyrathne

successfully completing the Diploma in Laboratory Technology in Chemistry programme conducted by the Institute, he was promoted to the post of Laboratory Technician in 2008. In 2016, Mr. Abeyrathna was promoted to the post of Education Assistant., Mr. Abeyrathna currently serves as the Educational & Service Officer of the Institute in which capacity he continues to discharge his duties with great responsibility, dedication and to the entire satisfaction of the Institute. In appreciation of over 20 years of devoted service to the Institute of Chemistry Ceylon, Mr. Hasantha Abeyrathne is awarded with the Long Service Award.

Mr. H. L. R. Hasantha Abeyrathna joined the Institute of Chemistry in 2005, as a Laboratory Assistant. After

### Mr. N. I. N. S. Nadarasa



**Mr. N. I. N. S. Nadarasa** graduated from the University of Colombo with a B.Sc. (Special) Degree in Chemistry in the year 1964. In the same year, he served the Department of Chemistry, University of Colombo as a temporary demonstrator. In 1966, he joined the Government Analyst's Department and retired as Deputy Government Analyst in 1999. While attached to the Government Analyst Department he obtained his M.Tech. (Master of Technology) in Environmental Pollution Science from Brunel University in UK.

Mr. Nadarasa has actively participated in the activities of the Institute of Chemistry as well, holding the post

of Asst. Treasurer (1984-1985), Treasurer (1982-1983), General Secretary (1985 - 1990), Vice President (1990 -1991, 1992 - 1993), Chairman/College of Past Presidents and was the President in the year 1991 - 1992. In addition, he served as the Chairman of the Admission and Ethical Practices Committee (1993 - 1999) and Chairman Awards Committee (1991- 1992). He represented the Institute in the Silver Jubilee Chemical Congress of the Malaysian Institute of Chemistry in 1992.

Mr. Nadarasa served as the Registrar from 1999 to 2021. Currently, he is working as the Senior Administrative Executive. He was involved in conducting all island examinations for Inter School Chemistry Quiz and Australian National Chemistry Quiz programmes. Mr. Nadarasa is currently the overall coordinator of the Australian National Chemistry Quiz programme. He received the Distinguished Service Award in 1995 in appreciation of the long years of dedicated service rendered to the Institute of Chemistry Ceylon.

In appreciation of over 25 years of devoted service to the Institute of Chemistry Ceylon, Mr. Nadarasa is awarded with the Long service award.

## CHEMISTRY IN SRI LANKA

Chemistry in Sri Lanka is a tri-annual publication of the Institute of Chemistry Ceylon and is published in January, May and September of each year. It is circulated among the members of the Institute of Chemistry and students of the Graduateship/DLTC course and libraries. The publication has a wide circulation and more than 500 copies are published. Award winning lectures, abstracts of communications to be presented at the annual sessions, review papers, activities of the institute, membership news are some of the items included in the magazine.

The editor invites from the membership the following items for publication in the next issue of the Chemistry in Sri Lanka which is due to be released in September 2025.

- Personal news of the members
- Brief articles of topical interests
- Forthcoming conferences, seminars and workshops
- Latest text books and monographs of interest to chemists

All publications will be subjected to approval of the 'Editorial and Publicity Committee' and the Council of the Institute of Chemistry Ceylon.

Further, prospective career opportunities for chemists, could be advertised in Chemistry in Sri Lanka at a nominal payment. The editor in charge welcomes suggestions from the members for improvement of the publication.

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## Chandrasena Memorial Award

Awarded for an exceptional research contribution of an original nature in the field of Organic Chemistry and/ or related areas such as Biochemistry, Pharmacognosy, Molecular Biology and Bioactivity studies.

#### Chandrasena Memorial Award - 2025

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**Professor Anoja Attanayake**, attached to the Department of Biochemistry, Faculty of Medicine, University of Ruhuna. She has served as a Biochemist for the past 15 years. She is the In-charge of the newly established Natural Products Research and Development Center at the Department of Biochemistry, Faculty of Medicine, University of Ruhuna. Prof Attanayake is engaged in research on Natural Products Chemistry, Biochemistry of metabolic diseases, Nutritional Biochemistry, and Nanodrug delivery systems, leading to several highimpact publications and collaborative projects with local and international institutions. She is a fellow of the Institute of Chemistry, Sri Lanka.

She underwent international training on Laboratory Animal Science in Netherlands, Fluorescence Microscopy, and Advanced Molecular Biology Techniques at ICGEB centers worldwide. She is a winner of 15 faculty, university, national, and international research awards for her exceptional research contribution towards the field of Biochemistry and Pharmacognosy, four national patents, took part in 2 commercialization agreements, and is a gold medalist in postgraduate research at the University of Ruhuna. She had delivered invited and plenary lectures at different international conferences. She supervised 5 PhDs, 2 MPhil projects up to date nurturing the next generation of scientists in Sri Lanka. She was the principal investigator of many research grants awarded by NRC, NSF, UGC, AHEAD DOR. Prof Attanayake has published 43 research articles in Science Citation Indexed/Expanded journals and 35 research articles in other peer-reviewed journals.

Further, she co-authored 8 book chapters, 138 abstracts, and 3 newsletter articles.Her H-index is 20 with nearly 1000 citations. She is a member of professional bodies, including SLAAS, SALAS, CBSL, and a Founder member of the Belt & Road Alliance for Traditional Chinese Medicine, University of Hong Kong. She is the President Elect of the College of Biochemists 2023-2025. She has played a pivotal role in enhancing biochemistry research and university education in Sri Lanka.

#### Abstract of Chandrasena Memorial Award - 2025

## Therapeutic Drug Leads from Sri Lankan Flora for Diabetes and Kidney Disease: From Bench to Bedside and Beyond

Anoja Attanayake

Professor in Biochemistry, Department of Biochemistry, Faculty of Medicine, University of Ruhuna Email: anojaattanayake@med.ruh.ac.lk

Natural products have been the basis of modern drugs, with more than half of all small-molecule drugs being based on natural products, and will remain an important source of future medicine and therapeutics. Nanotechnology has also proven to be instrumental in connecting the realms of natural products in the drug discovery process. Sri Lankan medicinal plants have a long history of use in traditional medicine practices to manage diabetes mellitus and kidney-related disorders. The research work presented here comprises comprehensive scientific studies that were conducted on therapeutic drug leads from Sri Lankan flora through preclinical, clinical, and advanced nanotechnology developments for diabetes mellitus and kidney disease. The *in vitro* and *in vivo* antidiabetic activity assessment of selected medicinal plant extracts (Spondias pinnata (L. F.) Kurz - Ambarella, Coccinia grandis L.- Kowakka and Gmelina arborea Roxb. -Et-demata, polyherbal formulation (composed of Garcinia quaesita Pierre-Rath goraka, seeds of Piper nigrum L.-black pepper, leaves of Murraya koenigii L. Sprengel-curry leaves, and cloves of Allium sativum L. -garlic), compound mixture (composed of garcinol, piperine, butyl oleate, pipnoohine, and bismurrayanimbine) were conducted in an animal model of diabetes. The results revealed the potent antidiabetic, antihyperlipidemic, and antioxidative activities of the selected medicinal plant extracts, polyherbal and compound mixture, both in vitro and in vivo, while ensuring in vivo safety. The bioactivity-guided isolation of the C. grandis leaves and the said polyherbal mixture resulted in antidiabetic compounds such as fucosterol, coccinoside C, garcinol, piperine, butyl oleate, pipnoohine, and bismurrayanimbine (novel compound). The results of computational docking studies further supported the in vitro antidiabetic activity of both fucosterol and coccinoside C. The encouraging results of preclinical studies on the assessment of C. grandis

extract paved the way to conduct a phase II clinical trial in newly diagnosed patients with diabetes mellitus. The safety-efficacy profile of the herbal capsule of C. grandis was established through a panel of biochemical and hematological parameters. Nephroprotective activity of selected medicinal plant extracts (Abelmoschus moschatus Medikus.- Kapu kinissa, Asparagus falcatus L. -Hathwariya, Barleria prionitis L. -Katu karandu, Gmelina arborea Roxb. -Et demata, Plectranthus amboinicus (Lour.) Spreng-Kapparawaliya, etc., and a polyherbal formulation (composed of A. moschatus, A. falcatus, and B. prionitis) were evaluated in a doxorubicin-induced nephrotoxicity model of kidney disease. Treatment with the selected plant extracts and the polyherbal formulation in doxorubicin-induced nephrotoxicity in Wistar rats caused significant nephroprotection through anti-inflammatory and antioxidant activities, with well-balanced in vivo safety. Biochemical results were further corroborated by histopathological and immunohistochemical findings. Medicinal plant extracts with previously proven antidiabetic activity were encapsulated into different nanodelivery systems, such as nanoliposomes, nanoemulsions, gelatin, etc. The encapsulated nanoformulations showed in vivo safety and a significant increase or preservation of antidiabetic activity. In conclusion, the research work presented here with intense devotion, research collaboration, cooperation, and an unwavering commitment for the past ten years would lead to shedding light on the road ahead in the development of therapeutic drug leads from the bench to the bedside and beyond in diabetes care and kidney health.

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## Kandiah Memorial Awards

Awarded for the best research contribution in Chemistry carried out by a postgraduate student registered for a postgraduate degree by either course work or/ and research at a Higher Educational Institute in Sri Lanka and for work carried out in Sri Lanka, with the exception of special analysis that cannot be done in the country. Such results should be less than 20% of the findings from the work. Sandwich programs carried out partially abroad do not qualify for the award.

## • Kandiah Award for Basic Chemistry For research predominately in basic Chemistry (Organic, Inorganic, Physical, and Analytical).

#### Kandiah Award for Applied Chemistry

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For research in Chemistry related areas such as polymer, food, biochemistry, biotechnology, where interdisciplinary research is involved and provided that chemistry has a central role and comprises at least 50% of the content.

#### Kandiah Memorial Graduateship Award

For the best piece of research in the Chemical Sciences carried out by a Graduate Chemist of the College of Chemical Sciences/Institute Chemistry Ceylon registered with a Higher Education Institute for a Post Graduate Degree.

## Kandiah Memorial Graduateship Award - 2025



Latheesha Abeywardana obtained her Graduateship in Chemistry from the College of Chemical Sciences, Institute of Chemistry Ceylon, and received the Mr & Mrs K. Sivarajah and Family Award for overall excellence in chemistry practicals in 2013. She also served as a graduate Teaching Assistant at the Institute of Chemistry Ceylon for two years. She subsequently completed a Postgraduate Diploma in Analytical Chemistry at the University of Colombo and an MPhil in Nano and Advanced Technology at the Sri Lanka Institute of Nanotechnology. Her MPhil research, titled "Next Generation Plant Nutrient Delivery System Based on Modified Hydroxyapatite Nanoparticles," was recognized with the National Science Foundation SURSED Award (Sri Lanka) in 2023 and resulted in publications in three peer-reviewed international journals and presentations at three international conferences.

Latheesha was later awarded a postgraduate research scholarship to pursue her PhD at Deakin University, Australia, where she is currently investigating "Electrospun Nanoencapsulation of Iron and Vitamin A for Edible 3D Printing." Her work focuses on addressing the limitations associated with the co-delivery of iron and vitamin A. In 2024, she received the Advanced Materials Best Poster Award at the International Conference on Nanoscience and Nanotechnology held in Melbourne. Latheesha is currently in the third year of her PhD and is expected to complete her studies in 2026.

#### Abstract of Kandiah Memorial Graduateship Award - 2025

## Next Generation Plant Nutrient Delivery Systems based on modified hydroxyapatite nanoparticles

Latheesha Abeywardana

Institute for Frontier Materials, Deakin University, Australia Email: lsa.a@live.com

Deficiencies in both macro and micro plant nutrients during the early stages of plant growth can significantly hinder plant development, ultimately leading to reduced agricultural yields. Traditional fertilizers often struggle with low solubility, nutrient leaching, and inefficiency, making it essential to explore innovative solutions. Nanotechnology has emerged as a promising tool for enhancing agricultural productivity, offering controlled and efficient nutrient delivery. Among various approaches, functionalized seed coatings capable of precise nutrient release have gained significant scientific interest.

This study focused on developing a smart seed coating designed to supply essential nutrients—zinc (Zn), phosphorus (P), and nitrogen (N)—at the critical early growth stage of plants. Modified hydroxyapatite (HA) nanoparticles were chosen as the nutrient carrier due to their biocompatibility, structural adaptability, and ability to improve nutrient bioavailability. The research was structured around several key objectives: the synthesis and structural characterization of Zn-doped HA/urea nanoparticles, elucidation of their chemical properties, optimization of Zn doping and urea modification, development of a compatible seed coating for Zea mays (corn) seeds, and evaluation of its impact on seed germination and growth.

To achieve these objectives, a one-pot in situ sol-gel method was employed to synthesize a nano-seed coating incorporating Zn-doped HA/urea nanoparticles. The resulting material featured a phase corresponding to parascholzite, confirming successful zinc incorporation into the hydroxyapatite structure. Characterization studies validated the formation of modified hydroxyapatite nanoparticles with lattice shrinkage, indicating structural changes due to Zn doping and urea modification. The developed nano-seed coating demonstrated improved seed germination, plant development, and crop yield in Zea mays. Its ability to deliver nitrogen, phosphorus, and zinc in a controlled manner positions it as a viable alternative to traditional fertilizers. The hydroxyapatite-based nanoparticles effectively addressed key challenges in conventional fertilizers, such as low phosphorus solubility, nitrogen loss due to volatilization, and the high cost of zinc fertilizers.

This study highlights the potential of hydroxyapatite nanoparticles as a macro-micro plant nutrient carrier, paving the way for a sustainable and efficient fertilization strategy. The developed nano-seed coating represents a futuristic approach to enhancing agricultural productivity while minimizing environmental impact. Furthermore, this research opens new avenues for investigating metal-doped hydroxyapatite nanoparticles for broader agricultural applications.

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## Professor M. U. S. Sultanbawa Award for Research in Chemistry

Awarded for the best research paper presented at the Annual Sessions of the Institute of Chemistry Ceylon, for the unique, distinguished and significant contribution made to the cause of Science, Chemistry, Education and Research in Sri Lanka.

### Professor M. U. S. Sultanbawa Award for Research in Chemistry - 2024



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**Piumika Yapa** is a researcher specializing in nanomedicine, antimicrobial materials, and advanced drug delivery systems. She is currently pursuing her Ph.D. in Chemistry at the University of Sri Jayewardenepura under the supervision of Prof. Imalka Munaweera, Dr. Laksiri Weerasinghe, and Prof. Manjula Weerasekera. Her doctoral research focuses on the development of electrospun hybrid nanofibrous membranes reinforced with multimetallic nanohybrids for antimicrobial applications, with a strong emphasis on addressing antimicrobial resistance and enhancing personal protective technologies.

Piumika holds a Bachelor of Pharmacy (Hons) from the University of Sri Jayewardenepura and a Postgraduate Diploma in Laboratory Animal Sciences from the University of Colombo. Her research contributions include multiple peer-reviewed journal publications, national and international conference presentations, several book chapters, and a co-authored book on nanotherapeutics. She has received numerous awards for her research excellence, including several first-place honors for outstanding oral presentations at national and international scientific conferences. She has also been involved in interdisciplinary projects exploring the biomedical potential of inorganic-nanohybrid materials, including antimicrobial formulations and self-sterilizing coatings. She currently serves as a Lecturer in Pharmaceutical Sciences at the Department of Pharmacy and Pharmaceutical Sciences, Faculty of Health Sciences, CINEC Campus, Sri Lanka.

Mr. Yapa will be awarded the Professor M. U. S. Sultanbawa Award for Research in Chemistry for the presentation of her research on "Multimetallic Silica Nanohybrids Incorporated Nanofiber Membrane for Potential Synergistic Antibacterial Applications" in 2024.

#### Professor M. U. S. Sultanbawa Award for Research in Chemistry - 2024

## Multimetallic Silica Nanohybrids Incorporated Nanofiber Membrane for Potential Synergistic Antibacterial Applications

Piumika Yapa<sup>1</sup>, Imalka Munaweera<sup>1\*</sup>, Manjula M. Weerasekera<sup>2</sup>, Laksiri Weerasinghe<sup>1</sup>

<sup>1</sup>Department of Chemistry, Faculty of Applied Sciences, University of Sri Jayewardenepura, Nugegoda (10250), Sri Lanka.

<sup>2</sup>Department of Microbiology, Faculty of Medical Sciences, University of Sri Jayewardenepura, Nugegoda (10250), Sri Lanka.

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The fatal pandemics and microbial infections have been sliding into our lives, and the necessity for improved safeguards against microbial threats is perhaps more critical than ever. Gloves and masks, diapers, sanitary napkins, wound dressings, and other PPEs have emerged as new weapons to shield human health in the post-new normal era. The age-old adage, "Prevention is better than cure," could not have been more appropriate when conversing with the area of public health. PPEs, hygiene products, and wound care products help protect people from pathogens but are also reservoirs of infection at the same time. There are limitations to conventional antimicrobials because traditional antiseptic measures like antibiotics provide prevention care but in the process are faced with challenges like antibiotic resistance, their cost, and availability.

Enter the breakthrough research of a new silica nanohybrid material capable of inhibiting bacterial and fungal growth and development which poses a high resistance challenge to humanity and is hence affordable and easily assessable. This flexible material can be readily incorporated into the polymer membranes and thus has ready applicability in PPE, personal care items, and wound care products. The research that underpins this kind of innovation concentrates on the enhancement of a multimetal-doped silica nanoparticle (SiNP) matrix. A sol-gel process yields a material that has a wide range of antimicrobial effects due to the embedding of copper, silver, and cobalt into a silica network. It is seen that every metal nanoparticle has a certain kind of action against different microorganisms; and silver and copper are effective against different types of bacteria, whereas cobalt is more effective against fungi. Altogether, these metals improve the synergistic antimicrobial activity

of the material and give it protection against a broad spectrum of pathogens including gram-positive and negative bacteria, yeast type, and filamentous type fungus.

The fact that this material could eradicate both bacteria and fungi sets it apart as a very useful material because most antibiotic-based substances usually have the proclivity to kill either the bacteria or the fungi but not both. Further, this material does not operate in a way that eliminates microbes immediately but rather releases reactive oxygen species (ROS) that interfere with the cell walls of microbes killing them in the process. This mechanism assists in avoiding the development of resistance which is a common issue associated with normal antibiotics.

The most substantial benefit of this silica nanohybrid material is that it has applications in virtually any product touched by consumers. Because its incorporation into polymer membranes does not alter the structural characteristic of the PPE, the nanohybrid can be easily implanted into masks and gloves, diapers sanitary napkins, and wound dressings. It can be seen from this that unlike commonly used antibiotics this antimicrobial layer is not only a cost-effective product but also has the capacity to be manufactured in large quantities to address the needs of the growing healthcare systems across the world.

What makes this innovation especially interesting is its ability to work as a solution to the problem of poor healthcare facilities. Since presently available antimicrobials are very expensive, it becomes difficult for many population groups, especially those in low and middle-income countries to afford a protective barrier against infections. The vision for this new nanohybrid is to make protection from diseases accessible to all on a global scale while preventing the over-consumption of resources inherent to existing premium products.

The development of this antimicrobial material relies on a straightforward yet effective process: the sol-gel method. This synthesis technique makes it possible to dope metal into the silica network sufficiently and generate highly porous nanoparticles that are ideal for cargo loading. The process is simple, and since it is very cost-effective, it is possible to implement large-scale production of the product. The mechanism of these metal-doped silica nanoparticles allows for the development of antimicrobial layers in textiles or polymer membranes once synthesized and incorporated.

These nanohybrids have been tested against a host of bacteria and fungi that are generally found to be resistant to many conventional anti-bacterial products and the test results have been very positive. In vitro studies showed that the investigated material possesses antifungal and antibacterial activity with low MIC values, as well as fungicidal and bactericidal effects. The nanohybrids have also been demonstrated to be non-irritation and can hence be used in products such as diapers, sanitary towels, and bandages. Moreover, there is a huge scope for the implementation of this technology. Not only is it a more environmentally friendly and cost-effective way of tackling microbial infection but it also tick all the boxes for the paradigms in unforeseen future public health emergencies. In the case of a future pandemic, flexibility to increase the production of antimicrobial PPE and hygiene products could be the key to eradicating the infection.

Also, the process of synthesizing the nanocomposite is relatively straightforward, which makes cellulose acetate nanocomposite an ideal material for manufacturers, who would like to incorporate as antimicrobial feature to the products by the simple technique "electrospinning", without reaching upon complicated and costly technologies. Thus, the approach with the ability to be used for a variety of industries, from healthcare to consumer goods, the multimetal-doped silica nanoparticle composite can become a staple in the daily lives of people at some point in the future.

This enhanced inexpensive and easily available antimicrobial membrane seems to be a giant step

towards controlling infectious diseases. As seen now, this discovery can enhance the state of public health around the world since it affords the combating means of various kinds of existing protective garments and other products, safe for individuals and the environment. Moving forward as we are confronted with new and emerging health threats, these innovations will be increasingly instrumental in anyone receiving the kind of security to prevent illness across geographic and socioeconomic space. Consequently, as the world continues to look for avenues through which they can count on in future pandemics and outbreaks, such an antimicrobial nanohybrid material for surfaces might well be the best bet in the world for averting the spread of diseases across the globe.

#### References

- Yapa PN, Munaweera I, Sandaruwan C, Weerasinghe L, Weerasekera MM. Metal doped silica nanohybrids with extensive bacterial coverage for antibacterial applications exhibit synergistic activity. *Biomater Adv.* 2024;157(213753):213753. http://dx.doi. org/10.1016/j.bioadv.2023.213753
- Yapa P, Munaweera I, Weerasekera MM, Weerasinghe L, Sandaruwan C. Potential antifungal applications of heterometallic silica nanohybrids: A synergistic activity. *Biomater Adv.* 2024;162(213930):213930. http://dx.doi.org/10.1016/j.bioadv.2024.213930
- Yapa P, Munaweera I, Weerasekera MM, Weerasinghe L. Synergistic antimicrobial nanofiber membranes based on metal incorporated silica nanoparticles as advanced antimicrobial layers. *RSC Adv.* 2024;14(46):33919-40. http://dx.doi. org/10.1039/d4ra05052e
- Anjum S, Ishaque S, Fatima H, Farooq W, Hano C, Abbasi BH, et al. Emerging applications of nanotechnology in healthcare systems: Grand challenges and perspectives. *Pharmaceuticals* (Basel) [Internet]. 2021;14(8):707. Available from: http:// dx.doi.org/10.3390/ph14080707
- 5. Yapa PN, Munaweera I, Weerasekera MM, Weerasinghe L. Nanoarchitectonics for synergistic activity of multimetallic nanohybrids as a possible approach for antimicrobial resistance (AMR). *J*

#### The Tri-Annual Publication of the Institute of Chemistry Ceylon

*Biol Inorg Chem.* **2024**;29(5):477–98. http://dx.doi. org/10.1007/s00775-024-02066-w

Wahab S, Salman A, Khan Z, Khan S, Krishnaraj C, Yun S-I. Metallic nanoparticles: A promising arsenal against antimicrobial resistance-unraveling mechanisms and enhancing medication efficacy. *Int J Mol Sci.* 2023;24(19):14897. http://dx.doi.

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org/10.3390/ijms241914897

 Kumarage S, Munaweera I, Kottegoda N. A comprehensive review on electrospun nanohybrid membranes for wastewater treatment. *Beilstein J Nanotechnol.* 2022;13:137–59. http://dx.doi. org/10.3762/bjnano.13.10

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## CCS Researcher of the Year Award

Awarded annually to a full time internal academic of the College of Chemical Sciences, Institute of Chemistry Ceylon, for the most outstanding contributions to scientific research in the course of a particular year. The criteria for the evaluation of the awardee includes peer-reviewed scientific publications, including research articles, review articles, and book chapters, conference presentations and Web of Science citations garnered throughout the course of the year.

## CCS Researcher of the Year Award - 2025



**Professor Gobika Thiripuranathar** obtained her Graduateship in Chemistry qualification with firstclass honors from the College of Chemical Sciences, Institute of Chemistry Ceylon, and topped the batch and awarded the Shireen Jayasuriya Memorial Gold Medal in 2006. In 2008, she received both the Overseas Research Student Award Scholarship and a Heriot-Watt University Scholarship to pursue her PhD at Heriot-Watt University in Scotland, where her research focused on polyhedral boron cluster chemistry. Dr. Gobika has an impressive research record, with 33 peer-reviewed publications, 11 book chapters, and 60 communications, with over 1250 citations and an h-index 18. She is the proud recipient of the CCS Best Researcher Award for three consecutive years, 2021, 2022 and 2023. Her research interests include the sustainable production of nanomaterials from agricultural wastes and underutilized resources from Sri Lanka, with a focus on value addition and resource utilization. Professor Gobika is a member of the internal academic staff at the College of Chemical Sciences, Institute of Chemistry Ceylon. 54th Annual Sessions & 84th Anniversary Celebrations of the Institute of Chemistry Ceylon

## Theme Seminar on

## **Chemistry for Quality Life**

Date : 17.06.2025Venue : Centre for Banking Studies, Rajagiriya, Sri Lanka

## Programme

8.15 a.m.	Registration and Refreshments
9.00 a.m.	Welcome Address
	Prof. Janitha A. Liyanage
	President, Institute of Chemistry Ceylon
9.15 a.m.	Molecules to Machines: The Convergence of Natural & Engineering Sciences - A Blueprint for
	Innovations
	Prof. (Dr.) Saranjit Singh
	Vice Chancellor, KIIT DU & Professor, School of Mechanical Engineering, Bhubaneswar, Odisha, India
10.00 a.m.	Rapid Detection of $\beta$ -Lactamase Expressing Antibiotic Resistant Bacteria
	Prof. Uday Maitra
	President, Chemical Research Society of India
	Department of Organic Chemistry, Indian Institute of Science, Bangalore, India
10.50 a.m.	Modulation in the Structure, Dynamics, and Enzymatic Activity of an Ordered Protein β-Lactoglobulin through Liquid-Liquid Phase Separation
	Prof. Saptarshi Mukherjee
	Department of Chemistry, IISER Bhopal, India
11.35 a.m.	Metal Organic Framework Based Triboelectric Nanogenerator for Powering Electronics
	Prof. Rojalin Sahu
	KIIT DU, Patia, Bhubaneswar, Odisha, India
12. 25 p.m.	Vote of Thanks
12.40 p.m.	Lunch

## Theme Seminar Chemistry for Quality Life

**Theme Seminar** 

## Molecules to Machines: The Convergence of Natural & Engineering Sciences – A Blueprint for Innovations

Saranjit Singh

Vice Chancellor, KIIT DU & Professor, School of Mechanical Engineering, Bhubaneswar, Odisha-751024, India Email: ssingh@kiit.ac.in

The merging of natural and engineering sciences, known as "Convergence Science," integrates methodologies from multiple disciplines to address complex challenges. Recent advancements in chemical synthesis and molecular engineering have enabled the design of functional materials with tailored properties such as conductivity, mechanical strength, and thermal resistance. These materials are vital for next-generation applications, including energy storage systems like solid-state batteries, electronics, lightweight structural composites in aerospace, and high-performance coatings. The integration also extends to medicine, exemplified by hydrogels used in tissue engineering. A notable example is the synthesis of tritium, a radioactive isotope for self-luminous lighting in aircraft. Other advancements include propellant materials designed

for controlled combustion and flame-retardant materials for fire safety. In manufacturing, ionic liquids are increasingly used as cutting fluids due to their low volatility and superior performance compared to traditional fluids. Additionally, smart materials like shape-memory alloys and stimuli-responsive polymers highlight the role of chemical science in enhancing mechanical adaptability. Overall, this convergence fosters innovative solutions and the development of new products and services.

#### Keywords:

Convergence Science, Functional Materials, Interdisciplinary Innovation



**Prof.** (Dr.) Saranjit Singh completed his Ph.D. (Production Engg) from BIT Mesra, Ranchi, M.Tech. (Production Engg) from IIT Varanasi (Formerly IT BHU) and B.E. (Mechanical Engg) from Savitribai Phule Pune University. His teaching & research areas of interest are material processing technologies, metal forming of sintered, cellular, foam, polymer and metal matrix composites, competitive manufacturing strategies, cleaner manufacturing technologies, DFX methodologies, quality engineering and quality management. He had guided 5 Ph.D scholars and 25 Master's Dissertation and had published / presented more than 100 research articles in the international & national journals, conferences and seminars. He has published 3 books in the area of material

processing technologies and is also Fellow of Institution of Engineers (India). He served as Director (Industry Engagements) and Dean (Training & Placements) since 2011 at KIIT. He is a Former Dean of School of Mechanical Engg at KIIT from 2009 to 2011. Prior to this, he served BIT Mesra, Ranchi as Assoc. Professor in Dept. of Production Engg. Currently, he is also Professor at School of Mechanical Engg, KIIT.

#### Theme Seminar

## Rapid Detection of β -Lactamase Expressing Antibiotic Resistant Bacteria

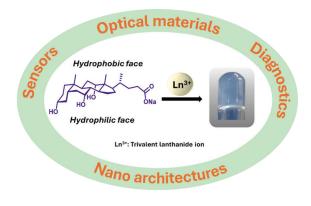
#### Uday Maitra

Department of Organic Chemistry, Indian Institute of Science, Bangalore 560012, India E-mail: maitra@iisc.ac.in

Almost 15 years ago, we discovered a facile method to enhance the luminescence from lanthanides through the self-assembly of multiple components in a metallohydrogel. Using this strategy, we have developed a masked sensitizer ("*pro*-sensitizer") based protocol for sensing enzymes and a few small molecules.

In this lecture, I will present our recent work on the rapid detection of  $\beta$  lactamase expressing bacteria. This work, initially done both with purified serine and metallo  $\beta$ -lactamases, was extended to clinical isolates of both resistant and non-resistant bacteria. We have demonstrated that unlike the "Gold standard" bacterial culture taking 1-3 days, our method could detect  $\beta$ -lactam antibiotic resistant organisms in about six hours, that too using an inexpensive portable device developed in our group. We followed up this work with simulated UTI samples which produced very

encouraging results which may lead to practical usage in a pathological laboratory.





**Prof. Uday Maitra** is a renowned Indian organic chemist and President of the Chemical Research Society of India. He is currently an Honorary Professor and INSA Senior Scientist at the Indian Institute of Science (IISc), Bangalore. His research focuses on supramolecular chemistry, including hydrogels, photoluminescent sensors, and bio-relevant molecular recognition. A recipient of the Shanti Swarup Bhatnagar Prize, he is also a Fellow of the Indian Academy of Sciences and the Indian National Science Academy.

*Education:* MSc IIT Kanpur; PhD Columbia University, New York (Prof. Ronald Breslow); Postdoctoral research University of California at Berkeley (Prof. Paul Bartlett).

Area of Research: Hydrogels, hybrid materials and photoluminescent sensors. Low cost, paper based photoluminescent sensors for a variety of analytes of biological interest. I am also greatly interested in Chemistry outreach programs.

*Major Recognition/Awards:* Elected fellow of the Indian Academy of Sciences and the Indian National Science Academy; Titular Member of the CCE of the IUPAC; President of the Chemical Research Society of India (CRSI).

#### Theme Seminar

## Modulation in the Structure, Dynamics, and Enzymatic Activity of an Ordered Protein β-Lactoglobulin through Liquid-Liquid Phase Separation

#### Saptarshi Mukherjee

Department of Chemistry, IISER Bhopal, Madhya Pradesh 462066, India Email: saptarshi@iiserb.ac.in

Bimolecular condensates formed through liquid-liquid phase separation (LLPS) of proteins, polypeptides, and nucleic acids have garnered significant research of late.1-3 Despite valuable contributions of prior research, there is untapped potential in exploring the influence of phase separation on the conformational dynamics and enzymatic activities of native proteins. Herein, we investigate the LLPS of β-Lactoglobulin  $(\beta$ -LG), a non-intrinsically disordered protein, under crowded conditions.<sup>4</sup> In-depth characterization through spectroscopic and microscopic techniques revealed the formation of dynamic liquid-like droplets, distinct from protein aggregates, driven by hydrophobic interactions. Our analyses revealed that phase separation can alter structural flexibility and photophysical properties. Importantly, the phaseseparated β-LG exhibited efficient enzymatic activity as an esterase; a characteristic seemingly exclusive to β-LG droplets.<sup>4</sup> Further investigation into the catalytic mechanism suggested the involvement of specific amino acid residues, rather than general acid or base catalysis. Our study delineates the understanding of protein phase separation and insights into the diverse catalytic strategies employed by proteins. It opens exciting possibilities for designing functional artificial compartments based on phase-separated biomolecules.

#### **References:**

- M. Mimura, S. Tomita, Y. Shinkai, T. Hosokai, H. Kumeta, T. Saio, K. Shiraki and R. Kurita, *J. Am. Chem. Soc.*, **2021**, *143*, 9849.
- 2. R. S. Fisher and S. Elbaum-Garfinkle, *Nat. Commun.*, **2020**, *11*, 4628.
- A. Patel, H. O. Lee, L. Jawerth, S. Maharana, M. Jahnel, M. Y. Hein, S. Stoynov, J. Mahamid, S. Saha, T. M. Franzmann, et al., *Cell*, 2015, *162*, 1066.
- S. Rai, S. Pramanik and S. Mukherjee, *Chem. Sci.* 2024, 15, 3936.



**Dr. Saptarshi Mukherjee** is presently a Professor at the Department of Chemistry, Indian Institute of Science Education and Research (IISER) Bhopal. He did both his BSc and MSc from Jadavpur University and carried out his doctoral research at the Indian Association for the Cultivation of Science, Kolkata under Professor Kankan Bhattacharyya on Time-Resolved Laser Spectroscopy. He then moved to the Bowling Green State University, Ohio for his post-doctoral research with Professor H. Peter Lu on Single Molecule Spectroscopy. He returned to India in late 2008 and joined the Department of Chemistry IISER Bhopal as an Assistant Professor where he still continuing.

Professor Mukherjee's research interests include ultrafast and single molecule spectroscopy of luminescent metal nanoclusters and self-assembled systems having biological relevance. He is the recipient of the INSA Young Scientist Award, CRSI Young Scientist Award, CRSI Bronze Medal and has been a Core and Founding Member of Indian National Young Academy of Sciences (INYAS). Professor Mukherjee is a Fellow of the Indian Academy of Sciences, Bangalore, the National Academy of Sciences, Allahabad, and a Fellow of the Royal Society of Chemistry. He is a Senior Editor of Chemical Physics Impact, a journal published by Elsevier.

He has also served IISER Bhopal as its first Deputy Director.

#### Theme Seminar

## Metal Organic Framework Based Triboelectric Nanogenerator for Powering Electronics

Rojalin Sahu

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Harnessing mechanical energy from the surroundings shows significant promise as a power supply for micro and nanoscale devices. The functionality of the triboelectric nanogenerator (TENG) is based on the principles of triboelectrification and electrostatic induction. Traditionally investigations on triboelectricity have been limited to metals and polymers. Therefore, it is necessary to expand the limits including other possible materials for triboelectricity . In this study, we synthesized a zeolitic imidazole framework (ZIF-67) using a solvent-assisted method at room temperature and its structural and chemical properties were investigated. Using additive manufacturing, a S-shaped TENG device in vertical contact mode was constructed. Here, ZIF-67 served as the positive triboelectric layer, while Teflon/PDMS served as the negative triboelectric layer. The multi-unit S-TENG device was used for selfpowered recognition of different gaits through digital signal processing. The device based on ZIF-67 and Teflon produced a voltage of 118 V, a current of 1.7 mA, and a power density of 15 mW cm<sup>2</sup> at a load resistance of 50 M $\Omega$ . By capturing the gait patterns of diverse volunteers, the S-TENG device assisted in accurately identifying various gaits to mitigate the risk of falls and injuries, particularly among children wearing flip flops equipped with the S-TENG technology while playing in a park. Furthermore, it was employed to charge a commercial capacitor to power a wristwatch and was attached to a robotic gripper for object identification.

**Keywords:** Metal organic framework, Triboelectric nanogenerator, Power Source, Solvothermal

#### **References:**

- B.C. Dhal, S. Hajra, A. Priyadarshini, S. Panda, V. Vivekananthan, J. Swain, S. Swain, N. Das, R. Samantray, H.J. Kim, R. Sahu\*, *Energy Technology*. 2024, 2400099.
- S. Hajra, M. Sahu, A.M.Padhan, J.Swain, B.K.Panigrahi, H.G. Kim, S. W. Bang, S. Park, R. Sahu\*, H.J. Kim\*. A new insight into the ZIF-67 based triboelectric nanogenerator for self-powered robot object recognition. *Journal of Materials Chemistry C.* 2021; 9(48):17319-30.



**Dr. Rojalin Sahu** is currently working as a Professor in the Department of Chemistry and Head, Central Research Facility, K-innovation at KIIT deemed to be University, Bhubaneswar. She is heading the Chemical Research Society of India (CRSI) and SMC Bhubaneswar Chapter. She has completed her M.Sc. and M.Phil. (Utkal University), PhD (IIT Guwahati). She is recently featured among 75 women researchers in STEAM by the Office of the Principal Scientific Advisor to the Government of India in partnership with Red Dot Foundation, British High Commission. She has been honoured with the prestigious title of Fellow of the Royal Society of Chemistry (FRSC), United Kingdom, in recognition of her contributions to materials science research. She is the recipient of

SMC Bronze medal, young researcher award by TEEKA foundation, Best staff award by KIIT. Most notably, she has been qualified Radiological Safety Officer (RSO) by BARC, Mumbai. She has been the lead Investigator of a number of externally funded projects (DST, DBT, ICMR, UGC-DAE-CSR, DRDO, Ministry of Mines and BRNS). She has successfully conducted many national and international conferences as convener. She is also a NABL trained officer for Chemical Testing Laboratories. Her basic areas of research are synthesis and characterization of new coordination compounds, Metal Organic Frameworks and Covalent Organic Frameworks for biomedical, environmental and energy application.

## 54<sup>th</sup> Annual Sessions of Institute of Chemistry Ceylon Technical Sessions 2025

8.00 am - 4.30 j	pm 18 <sup>th</sup> June 2025	Adamantane House, Rajagiriya
8.00 am - 9.00 am	Arrival of Guests	
9.00 am - 9.20 am	Kandiah Memorial Graduateship Award	l Lecture
	Ms. W. A. D. Latheesha S. Abeywardar	ia
	Institute for Frontier Materials, Deakin U	Iniversity, Australia
9.20 am - 9.40 am	Professor M. U. S. Sultanbawa Award for	r Research in Chemistry
9.40 am - 10.00 am	Refreshment Break	

## Presentations of Prof. M. U. S. Sultanbawa Award for Research in Chemistry

Time	Title	Authors	Abstract No.
9.20 am - 9.40 am	Chitosan-Stabilized Silver Nanoparticles: Molecular Dynamics Simulation on the Stability and <i>in-vivo</i> Interactive Toxicity with Cadmium on an Aquatic Model <i>Moina</i> <i>macrocopa</i>	M. T. R., Dahanayake J. N., and	2025_287

## Technical Sessions - 1

#### Session Chair: Prof. Suranga Wickramarachchi

Sub Theme: Nanotechnology

Venue: PPGL Siriwardene Auditorium

Time	Title	Authors	Abstract No.
10.00 am - 10.15 am	Formulation of <i>Psidium guajava</i> Linn essential oil encapsulated solid lipid nanoparticles and evaluation of its anti- inflammatory and antioxidant activity	M. G. C. Lakmali, H. I. C. De Silva	2025_289
10.15 am - 10.30 am	Investigation of catalytic properties of green synthesized copper oxide nanoparticles in Biginelli reaction	P. A. S. H. Perera, H. I. C. De silva	2025_290
10.30 am - 10.45 am	Evaluation of <i>Justicia adhatoda</i> Linn. extract-loaded layered double hydroxide nanohybrid for sunscreen applications	W. A. S. B. Gunaratne, H. I. C. De Silva	2025_291
10.45 am - 11.00 am	Antifungal efficacy of metallic silica nanohybrids embedded in hydrogel formulations for enhanced dermatological applications	P. N. Yapa, I. Munaweera, M. M. Weerasekera	2025_294
11.00 am - 11.15 am	Enhanced antimicrobial and anti- inflammatory properties of PCL metal- turmeric oleoresin and metal-curcumin nanohybrids	Dinithi Senanayake, Piumika Yapa, Sanduni Dabare, Manjula M. Weerasekera, Thusitha N. B. Etampawala, Maheshika Sethunga, Dinesh Attygalle, Shantha Amarasinghe, Imalka Munaweera	2025_297

11.15 am - 11.30 am	Harnessing the Power of Visible Light with GO-Ni-ZnO Nanohybrid Electrospun Polymeric Membranes for Improved Photocatalysis: A Focused Approach to Fabrication, Characterization, and Applications	Viraj Pasindu, Piumika Yapa, Sanduni Dabare, Imalka Munaweera, Thusitha Etampawala, Manjula M. Weerasekera, Dinesh Attygalle, Shantha Amarasinghe	2025_298
11.30 am - 11.45 am	Copper-zinc oxide nanohybrids for advanced antimicrobial and photocatalytic applications	Hasitha Herath, T. A. V. Pasindu Viduranga, Piumika Yapa, Imalka Munaweera, Upeka Samarakoon	2025_299
11.45 am - 12.00 noon	Synthesis of Cellulose Nanoparticles from Panicum maximum and their Application in Gas Filtration	A. H. M. Y. Nilmani, N. Priyantha, M. B. Wijesinghe	2025_304

## Session Chair: Dr Laksiri Weerasinghe

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Sub Theme: Nanotechnology	Venue: PPGL Siriwardene Auditorium

Time	Title	Authors	Abstract No.
1.00 pm - 1.15 pm	Evaluation of antibacterial activity in green synthesized chitosan–silver nanoparticles for therapeutic applications	O. W. Halwala and S. R. Wickramarachchi	2025_340
1.15 pm - 1.30 pm	Nano-crystalline hydroxyapatite from scales of the reef fish <i>Epinephelus</i> <i>malabaricus</i> (galkossa)	D. P. Rathu Gamathige, K. C. Weerasiri, and H. M. K. K. Pathirana	2025_324
1.30 pm - 1.45 pm	Analysis of malachite green adsorption on multiple coated graphite oxide/sand (M-GO/S) composite by incorporating isotherm and kinetic studies	K. A. V. Samod, K. A. D. D. Sakunthala, W. P. R. T. Perera, W. A. P. J. Premaratne, and J. A. Liyanage	2025_335
1.45 pm - 2.00 pm	Green synthesis of ZnO nanoparticles using the stem of <i>Murraya koenigii</i> and investigation of their photocatalytic activity	D. T. R. Perera, and K. C. Weerasiri	2025_338
2.00 pm - 2.15 pm	Development of dual-carrier CMC–PEG/ LDH nanocomposite hydrogel for the sustained release of <i>Mikania cordata</i> phytochemicals	N. Ananthalingam, C. D. Wijayarathna, and H. I. C. De Silva	2025_321

## Session Chair: Prof Dhammike Dissanayke

Sub Theme: Computational Chemistry

Venue: PPGL Siriwardene Auditorium

Time	Title	Authors	Abstract No.
3.00 pm - 3.15 pm	Altering bioavailability in curcumin derivatives: an <i>in-silico</i> study	W. P. D. Lakna, A. Mohomed, and A. P. P. Keerthi	2025_311
3.15 pm - 3.30 pm	Novel Curcumin Derivatives Loaded Chitosan Nanoparticles as Therapeutic Agents for Alzheimer's Disease: an <i>in-silico</i> Evaluation	A. K. M. Fernando and J. N. Dahanayake	2025_341

### The Tri-Annual Publication of the Institute of Chemistry Ceylon

3.30 pm - 3.45 pm	Effects of bisphenol A and its' substitutes on type 2 diabetes mellitus: an <i>in-silico</i> study	W. A. N. H. Wijesooriya and J. N. Dahanayake	2025_343
3.45 pm - 4.00 pm	Pomegranate phytochemical-loaded nanocarriers as therapeutic anti-cancer agents: an <i>in-silico</i> study	A. I. Nicholas and J. N. Dahanayake	2025_344

## Technical Sessions – 2

Session Chair: Prof Ireshika De Silva

Sub Theme: Natural Products / Organic Chemistry Venue: Level 05 Hall

Time	Title	Authors	Abstract No.
10.00 am - 10.15 am	Development of herbal tea from fruit peel of pomegranate cultivars grown in Sri Lanka	M. D. J. Mirando and M. K. B. Weerasooriya	2025_259
10.15 am - 10.30 am	Comparative analysis of nutritional and phytochemical properties of <i>Murraya</i> <i>koenigii</i> and <i>Micromelum minutum</i> cultivated in Sri Lanka	W. D. S. S. N. Ranasingha, K. A. D. D. Sakunthala, W. P. R. T. Perera, T. Abeysinghe, J. A. Liyanage, and W. A. P. J. Premaratne	2025_271
10.30 am - 10.45 am	Nutritional and phytochemical profiling of <i>Garcinia quaesita</i> dried fruit rinds: a comparative study of commercially available samples in Sri Lanka	U. L. P. Deepajith, K. A. D. D. Sakunthala, W. P. R. T. Perera, T. Abeysinghe, J. A. Liyanage and W. A. P. J. Premaratne	2025_273
10.45 am - 11.00 am	Development of a value-added pumpkin ( <i>Cucurbita spp.</i> ) and curry leaves ( <i>Murraya</i> <i>koenigii</i> ) instant soup mixture and its proximate analysis	W. P. K. K. de Silva and D. T. Abeysinghe	2025_277
11.00 am - 11.15 am	Antioxidant and photoprotective properties of <i>Flacourtia indica</i> fruit extract: fractionation, and application in lipstick formulation	D. M. M. D. Dasanayaka and C. S. K. Rajapakse	2025_282
11.15 am - 11.30 am	Antioxidant Activity, Phytochemical Screening and GC-MS Profiling of Some Tea Varieties of Sri Lanka	J. K. P. Malshika and E. M. R. K. B. Edirisinghe	2025_300
11.30 am - 11.45 am	Exploring bioactive compounds and antioxidant activity of selected Sri Lankan medicinal plants for skincare innovation	W. M. R. S. S. Werellagama and E. M. R. K. B. Edirisinghe	2025_312
11.45 am - 12.00 noon	Comprehensive physicochemical characterization and bioactivity assessment of Rajata Bhasma as a multi-target therapeutic agent	U. H. P. Jeewanthi, K. N. Seneviratne, S. Wickramarachchi, N. Jayathilaka, M. B. Chawda, R. V. Gudi, K. M. Bhapkar, and P. A. Paranagama	2025_330

Time	Title	Authors	Abstract No.
1.00 pm - 1.15 pm	Standardization and bioactivity evaluation of a distillate from a traditional herbal formula	Nilaksha Navod, K. N. Seneviratne, N. Jayathilaka, and P. A. Paranagama	2025_331
1.15 pm - 1.30 pm	Standardization, phytochemical profiling, and bioactivity evaluation of a traditional herbal tea bag formulation	Nilaksha Navod, K. N. Seneviratne, N. Jayathilaka, and P. A. Paranagama	2025_332
1.30 pm - 1.45 pm	Evaluation of the in vitro bioactive potential of <i>Salicornia brachiata</i> for therapeutic applications in metabolic disorders	K. G. S. Madushantha, K. N. Seneviratne, N. Jayathilaka, D. Perera, R. N. Attanayake, and P. A. Paranagama	2025_333
1.45 pm - 2.00 pm	Synergistic enhancement of <i>in-vitro</i> cell migration by ethuliacoumarin and stigmasterol from <i>Jeffreycia zeylanica</i> : A preliminary investigation using the response additive approach	W. M. P. Samarasinghe, G. M. K. B. Gunaherath, C. Ranasinghe and K. H. Jayawardana	2025_260
2.00 pm - 2.15 pm	α-Amylase Inhibitory Activity of Fractions Separated from The Seed Extract of <i>Syzygium cumini</i> (L.) Skeels	T. T. L. Fernando, M. S. T. Munasinghe, and H. I. C. De Silva	2025_293
2.15 pm - 2.30 pm	Synthesis and determination of <i>in-vitro</i> anti-urolithiatic activity of quinazolinone derivatives	U. B. P. M. Udapola, D.M.W.S. Dissanayake, and M. J. Gunaratna	2025_327

## Session Chair: Dr Dinusha Udukala Sub Theme: Natural Products / Organic Chemistry / Biochemistry

Venue: Level 05 Hall

## Technical Sessions – 3

Session Chair: Prof Hema Pathirana

Sub Theme: Analytical Chemistry

Venue: Level 04 Hall

Time	Title	Authors	Abstract No.
10.00 am - 10.15 am	Adsorptive removal of chromium (VI) from aqueous solutions using activated carbon derived from Calabash ( <i>Crescentia</i> <i>cujete</i> ) fruit shell	K. M. Senevirathna, and J. Prabagar	2025_276
10.15 am - 10.30 am	Determination of the antibiotic amoxicillin in milk	M. N. F. Salma, O. K. D. U. P Nishshanka, and D. T. Abeysinghe	2025_278
10.30 am - 10.45 am	Electrochemical Impedance Spectroscopy for Prediction of Corrosion Inhibition of CaO Nanoparticles toward Grade 202 Stainless-steel	M. H. N. Revon and N. Priyantha	2025_288
10.45 am - 11.00 am	Use of Aqueous Na <sub>2</sub> CO <sub>3</sub> Systems for Inhibition of Corrosion of Grade 202 Stainless-steel	P. D. T. A. Dewappriya, M. H. N. Revon and N. Priyantha	2025_292

## The Tri-Annual Publication of the Institute of Chemistry Ceylon

11.00 am - 11.15 am	Electrochemical Investigation of Thiamethoxam on Glassy Carbon Electrode	J. H. L. K. Jayasinghe and A. N. Navaratne	2025_302
11.15 am - 11.30 am	Enhanced Removal of Ni(II) from Contaminated Solutions by NaOH- modified Tea Waste	Chamith Manujaya and N. Priyantha	2025_305
11.30 am - 11.45 am	Quantitative analysis of morphology of microplastics in small pelagic fish species from the western and north-western coastal waters of Sri Lanka	N. K. D. M. P. Jayarathna, A. A. D. Amarathunga, D. S. M. De Silva, C. N. Walpita, and M. D. S. R. Maddumage	2025_307
11.45 am - 12.00 noon	Interpretation of Cr(III) adsorption by water hyacinth ( <i>Eichhornia crassipes</i> ) biosorbent through kinetics and isotherm analysis	A. P. N. H. D. Amarasinghe and N. Priyantha	2025_310

## Session Chair: Prof Namal Priyantha

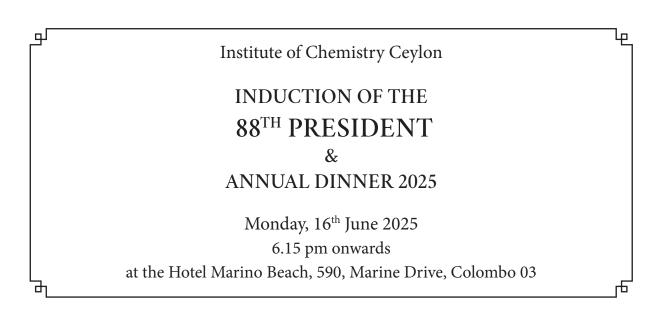
Sub Theme: Analytical Chemistry

Venue: Level 04 Hall

Time	Title	Authors	Abstract No.
1.00 pm - 1.15 pm	A study of microplastics present in edible salts in Sri Lanka	P. T. D. Pathirage, K. C. Weerasiri, and H. M. K. K. Pathirana	2025_309
1.15 pm - 1.30 pm	Assessment of microplastic pollution in water and sediment: a preliminary study in Uma-oya and Badulu-oya sub-catchments of the Mahaweli river, Sri Lanka	N. T. Chandana, D. S. M. De Silva, A. A. D. Amarathunga, N. D. Hettige, and H. A. C. C. Perera	2025_313
1.30 pm - 1.45 pm	Microplastics in Sri Lankan freshwater ecosystems: abundance, characterization, and sources in two major reservoirs	A. A. S. Lahiru, D. S. M. De Silva, A. A. D. Amarathunga, and S. R. C. N. K. Narangoda	2025_316
1.45 pm - 2.00 pm	Development of 8-hydroxyquinoline derivatives as fluorescence sensors for Zn <sup>2+</sup> detection	M. G. S. Raveesha, R. A. A. S. Ranasinghe, M. D. P. De Costa, and D. T. U. Abeytunga	2025_320
2.00 pm - 2.15 pm	Abundance and characterization of microplastics in <i>Dawkinsia filamentosa</i> inhabiting the Kothmale reservoir, Mahaweli upper catchment in Sri Lanka	H. N. L. Jayasekara, D. S. M. De Silva, A. A. D. Amarathunga, C. N. Walpita, and S. R. C. N. K. Narangoda	2025_322
2.15 pm - 2.30 pm	Development of plasma-activated coconut coir biochar for the efficient removal of rhodamine B, Cu(II), nitrate and ammonium ions from aqueous media	Sithira Ariyawansa, Didula Nawodya, Sharuka Akalanka, Ridma Sewwandi, Sehan Jayasinghe and Chandani Perera	2025_342

Time	Title	Authors	Abstract No.
3.00 pm - 3.15 pm	Determination of rainwater quality at selected locations in Kandy district	Kankanamge K.N.K., and Priyantha N.	2025_326
3.15 pm - 3.30 pm	A novel energy-efficient method to produce crystalline silica from burnt rice husk ash	N. G. H. J. Bandara, K. G. S. Madhushantha, C. R. De Silva, and C. N. Ratnaweera	2025_328
3.30 pm - 3.45 pm	Novel Zr(IV) and Hf(IV) – Schiff base complexes as white light photocatalysts for the degradation of methylene blue	S. Lilachjini, A. A. D. M. Adhikari, M. H. F. Amnah and C. V. Hettiarachchi	2025_329
3.45 pm - 4.00 pm	Investigation of curry leaves ( <i>Murraya koenigii</i> ) as a sustainable biosorbent for cadmium removal in aqueous solutions	R. P. D. S. Induwari, K. A. D. D. Sakunthala, W. D. S. S. N. Ranasingha, W. P. R. T. Perera, T. Abeysinghe, J. A. Liyanage, and W. A. P. J. Premaratne	2025_336
4.00 pm - 4.15 pm	Evaluation of <i>Garcinia quaesita</i> fruit rinds as a sustainable biosorbent for effective cadmium removal	R. U. Hettige, K. A. D. D. Sakunthala., U. L. P. Deepajith, W. P. R. T. Perera, T. Abeysinghe, J. A. Liyanage, and W. A. P. J. Premaratne	2025_337
4.15 pm - 4.30 pm	Electroanalytical detection of imidacloprid on stearic acid modified glassy carbon electrode	J. M. Hewagampalage and A. N. Navaratne	2025_325

## Session Chair: Prof Chandani Perera Sub Theme: Analytical Chemistry Venue: Level 04 Hall



## Abstracts of Research Papers to be presented at the 54<sup>th</sup> Annual Sessions 2025

Abstract No: 2025\_259

## Development of herbal tea from fruit peel of pomegranate cultivars grown in Sri Lanka

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Pomegranate (Punica granatum L., family Punicaceae), is used in folklore medicine for the treatment of various diseases. Its peel is a valuable waste rich with a diverse range of bioactive compounds bearing significant antimicrobial, antioxidant, and anticancer activities. This work aims to develop herbal tea using pomegranate peel, which is reported to possess high antioxidant activity. Kalpitiya hybrid(K), Daya(D), and Nimali(N) cultivars were used for the study. Dried peel powder (ppp) was prepared in tea bags and sachet packets and stored in the covered box at room temperature. Their Antioxidant capacity was monitored at every threeweek interval for 24 weeks. Consumer acceptability and microbial contaminant were also tested at end of 24th week. Tea prepared by tea bags were labelled as Kalpitiya hybrid (Kw), Daya (Dw), and Nimali (Nw). Tea prepared by sachets were labelled as Kalpitiya hybrid (Kws), Daya (Dws), and Nimali (Nws). The Observed total phenolic content (TPC) (mg GAE/g sample) was higher in Kws, Dws, and Nws than that of Kw, Dw, and Nw, respectively. Similarly, total flavonoid content (TFC) (mg CHE/g sample) was higher in Kws,

Dws and Nws than that of Kw, Dw, and Nw respectively. Ferric reducing antioxidant power (PFRAP) (mmol AAE/g sample) was higher in Kws, Dws, and Nws than that of Kw, Dw, and Nw, respectively. Also, the decline in TPC, TFC, and PFRAP values over a 6-month period is less in Kws, Dws, and Nws than in Kw, Dw, and Nw. Overall, consumer acceptability of all tea samples was at a moderate level. Microbial contamination was well below than the countable level. All these findings suggest that the antioxidant activity of herbal tea, prepared through a sachet, is higher than that prepared by a tea bag and safe to consume even over a 6-month period.

**Keywords:** Pomegranate peel; Herbal tea; Antioxidants; Anti-cancer.

#### *Abstract No: 2025\_260*

## Synergistic enhancement of *in-vitro* cell migration by ethuliacoumarin and stigmasterol from *Jeffreycia zeylanica*:

## A preliminary investigation using the response additive approach

<u>W. M. Priyantha Samarasinghe</u><sup>1,†</sup>, G. M. Kamal B. Gunaherath<sup>1\*</sup>, Chandani Ranasinghe<sup>1</sup> and Kithsiri Hector Jayawardana<sup>2</sup>

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Scratch wound assay (SWA) directed fractionation of the hexane extract of aerial parts of J. zeylanica led to the isolation of ethuliacoumarin (1) and stigmasterol (2). These two compounds exhibited enhanced invitro cell migration activity each at 12.5 µM (1-67.0% and 2-73.5%) compared to the negative control (20.1%) in SWA performed on Madin-Darby Canine Kidney (MDCK) cells. The interaction between 1 and 2 was studied by employing the response additive approach. In this method, the SWA was performed for compounds 1 and 2 separately at the doses lower than ED<sub>50</sub> and the dose pair combinations of compounds 1 and 2 in which the concentration of each is less than its  $ED_{50}$  value. The mean percent wound closures ( $E_{Observed}$ ) were determined for each dose pair combination. For each dose pair, the expected additive effect (E<sub>Expected</sub>) was determined by summing the mean percent wound closures observed for each compound when they were individually subjected to SWA at the corresponding doses in the combinations. The combination index (CI)

for each dose pair combination was calculated. It was found that the tested dose pair combinations showed significantly higher cell migration effect ( $E_{Observed}$ ) than the expected additive effect ( $E_{Expected}$ ) in which CI > 1. Therefore, the presence of ethuliacoumarin (1) and stigmasterol (2) in the hexane extract of aerial parts of *J. zeylanica* may contribute synergistically to its effective cell migration activity. Further studies with different pharmacological approaches/models are necessary to draw firm conclusions on the interaction between compounds 1 and 2.

#### Keywords:

Synergistic interaction, cell migration, ethuliacoumarin, stigmasterol, *Jeffreycia zeylanica* 

#### Acknowledgments:

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#### Abstract No: 2025\_271

## Comparative analysis of nutritional and phytochemical properties of *Murraya koenigii* and *Micromelum minutum* cultivated in Sri Lanka

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Curry leaves, native to Sri Lanka, Bangladesh, and India, are utilized as a flavoring agent and as a crucial component in Ayurvedic medicine. This study aims to compare the nutritional and phytochemical properties of Murraya koenigii and Micromelum minutum. Samples of both species were collected from domestic gardens in the Kurunegala district of Sri Lanka, which were of similar age. Standard AOAC techniques were used to estimate the proximate composition, while total phenol content (TPC), flavonoid content (TFC), and in vitro antioxidant activity were assessed. All experiments were conducted in triplicate, and statistical analysis was carried out using ANOVA followed by Tukey's pairwise comparisons. The results demonstrated notable differences in the proximate composition between the two species. M. minutum contained higher moisture  $(19.33 \pm 0.01\%)$  and protein content  $(18.00 \pm 0.01\%)$ . In contrast, M. koenigii showed significantly higher fat content ( $6.30 \pm 0.25\%$ ). Regarding phytochemical content, the ethanol extract of M. koenigii showed a higher flavonoid content (17.24  $\pm$  0.05 mg CE/g) compared to *M. minutum* (13.00  $\pm$  0.02 mg CE/g). The

ANOVA revealed a significant difference (p < 0.05) in total phenolic content, with M. koenigii having more than twice the TPC of the other species. Additionally, Tukey's test showed superior DPPH (2,2Diphenyl-1-picrylhydrazyl) radical scavenging activity in M. *koenigii* as evidenced by its lower IC<sub>50</sub> value (16.0  $\pm$ 0.9)  $\mu$ g/mL compared to *M. minutum* (18.9 ± 0.9  $\mu$ g/ mL). In conclusion, this study underscores the unique nutritional and phytochemical characteristics of both species. M. koenigii appears to be a better source of energy due to its higher fat content and exhibits remarkable antioxidant potential, enhancing its role in traditional medicinal applications. Furthermore, M. minutum serves as an excellent dietary source of protein. These findings highlight the complementary benefits of both species, suggesting their potential roles in nutrition and medicine.

#### Keywords:

*Murraya koenigii; Micromelum minutum;* Proximate analysis; Phytochemical analysis; Antioxidant activity.

#### *Abstract No: 2025\_273*

## Nutritional and phytochemical profiling of *Garcinia quaesita* dried fruit rinds: a comparative study of commercially available samples in Sri Lanka

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The fruit rind of Garcinia quaesita, commonly known as "Goraka" in Sri Lanka, has been utilized in Southeast Asia as a flavor enhancer and food preservative. This study compares the proximate composition and phytochemical properties, including in vitro antioxidant activity, of five different commercially available samples of dried G. quaesita rinds (assigned A-E) collected from the Panadura region, Sri Lanka, to minimize environmental variability. Four samples (A-D) were packaged under specific commercial brands with labeled containers, while sample E was a commonly retailed, unpackaged product without branding. Proximate composition, including fat content, crude protein, fiber, moisture, and ash, was analyzed using standard AOAC methods with slight modifications. Phytochemical evaluations included total flavonoid content (TFC), total phenolic content (TPC), and antioxidant activity. All measurements were triplicated, and statistical analysis was carried out using ANOVA followed by Tukey's HSD post-hoc test. Sample E exhibited the highest moisture content, indicating greater water absorption due to prolonged

atmospheric exposure. It also showed the highest fat content (10.29±0.40%), while B had the lowest  $(6.33\pm0.16\%)$ , with a significant difference (p<0.05). Sample A demonstrated significantly higher fiber and ash contents. Protein levels ranged from 3.09% to 4.60%. Sample E had the highest TFC (117.49±1.58 mg CE/g), with no significant difference between samples A and D. The TPC of A, E, and C showed slight variation, while samples B (52.66±0.83 mg GAE/g) and D (81.86±0.61 mg GAE/g) had significantly higher levels. Antioxidant activity, assessed by IC<sub>50</sub> from the DPPH (2,2-diphenyl-1-picrylhydrazyl) assay, followed the order A<E<B<D<C, with sample A (142.8±18.6 µg/mL) showing the highest and C (328.1±12.7 µg/ mL) the lowest activity. The results reveal notable variability in proximate and phytochemical profiles among G. quaesita products, likely due to differences in preparation and environmental exposure.

#### Keywords:

*Garcinia quaesita*, Proximate composition, Flavonoid content, Phenolic content, Antioxidant activity

# Adsorptive removal of chromium (VI) from aqueous solutions using activated carbon derived from Calabash (*Crescentia cujete*) fruit shell

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Heavy metal contamination, particularly from hexavalent chromium [Cr(VI)], poses a significant environmental and health hazard due to its toxicity and persistence in aquatic systems. Conventional Cr(VI) treatment methods are often costly, complex, and generate secondary pollutants, necessitating sustainable alternatives. This study investigates the potential of activated carbon derived from Calabash (Crescentia cujete) fruit shells as a low-cost, ecofriendly adsorbent for Cr(VI) removal from aqueous solutions. Activated carbon was prepared through controlled carbonization at 400 °C for 40 minutes using a muffle furnace, followed by chemical activation using H<sub>3</sub>PO<sub>4</sub>. The physicochemical properties of carbonized samples at various temperatures were analyzed to determine the optimum carbonization temperature. Batch adsorption experiments were conducted at room temperature (30 °C) and pH 2 to examine the effects of key operational parameters such as initial Cr(VI) concentration, adsorbent dosage, and contact time. The concentration of Cr(VI) in solutions was determined using a UV-Vis spectrophotometer at 542 nm with the 1,5-diphenylcarbazide method. Physicochemical characterization revealed that carbonization at 400 °C produced the optimal adsorbent, with the highest fixed carbon content (70.89%) and moderate ash

content (3.29%). Optimization results indicate that activation significantly enhances adsorption, with activated carbon achieving  $93.25 \pm 0.42\%$  removal at 1 ppm, compared to  $76.73 \pm 0.48\%$  for non-activated carbon and  $68.89 \pm 0.46\%$  for raw material of calabash fruit shell. Adsorption efficiency decreased at higher Cr(VI) concentrations. The optimal adsorbent dosage was 0.4 g, at which activated carbon, non-activated carbon, and raw material achieved higher removal efficiencies. Beyond this dosage, further increases yielded minimal additional removal. The optimal contact time was 60 minutes, where activated carbon, non-activated carbon, and raw material achieved removal efficiencies of  $93.14 \pm 0.50\%$ ,  $76.76 \pm 0.42\%$ , and 68.64  $\pm$  0.62%, respectively. By 60 minutes, removal efficiency had reached a near-optimal level, with only minor improvements thereafter. These findings suggest activated carbon from Calabash fruit shells is a promising, cost-effective, and sustainable alternative for Cr(VI) removal in wastewater treatment, contributing to environmental protection and resource recovery.

### Keywords:

Hexavalent Chromium, Adsorption, Activated Carbon, UV-Vis Spectrophotometry, Wastewater treatment.

# Development of a value-added pumpkin (*Cucurbita spp.*) and curry leaves (*Murraya koenigii*) instant soup mixture and its proximate analysis.

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A healthy diet for humans should include a variety of foods, prioritizing providing a variety of nutrients. Nowadays, soup is considered a good food supplement due to its ability to provide a variety of nutrients, hydration, and support for digestion. In the modern world, soup is now commercially available in the form of instant soup as an alternative to homemade soup. Pumpkins (*Cucurbita* spp.) are a nutritious food source, with essential vitamins, minerals, antioxidants, and carotenoids. In Sri Lanka, a significant portion of the pumpkin harvest is wasted, and therefore, we aimed to make an instant soup mix with pumpkin. Curry leaves (*Murraya koenigii*), black pepper (*Piper nigrum L.*), salt, and sweet potato (*Ipomoea batatas*) starch were used as other ingredients, creating a synergy that enhances both flavour and nutrition. The composition of the soup mix was selected via a sensory test, and the proximate analysis was done according to the AOAC standard methods. Moisture content was  $15.52\pm0.90\%$ , and the total ash content was  $11.67\pm0.54\%$ . The fat content of the soup mix was 0.97%. The protein content determined by the Kjeldahl method was  $2.17\pm1.53\%$ . The crude fibre content was 0.90% and the total carbohydrate content was 68.77%. These findings revealed promising results from the proximate analysis, highlighting the nutritional quality of the instant soup mix.

#### Keywords:

Pumpkin, Curry leaves, Sweet potato, Instant Soup Mix, Proximate analysis

*Abstract No: 2025\_278* 

# Determination of the antibiotic amoxicillin in milk

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Milk proteins are among the most essential constituents of milk in terms of biological and nutritional properties. The use of antibiotics in food-producing animals causes the subsequent deposition of these drug residues in milk. Therefore, the quality of milk can be impaired due to antibiotics, leading to serious health concerns worldwide and in Sri Lanka, including antibiotic resistance and other adverse effects. Since milk is a highly consumed product globally, it is essential to conduct thorough testing to detect and quantify these residues to guarantee their safety. Therefore, this study aimed to determine the residue level contamination of amoxicillin, a commonly utilized veterinary antibiotic, in selected raw and processed milk samples and assess their human health risks. The processed, pasteurized, and raw milk samples were collected from local markets and stored at -20 °C till further analysis. Amoxicillin was extracted by an acetonitrile-methanol-distilled water (40:20:20) solvent system, and further analysis was conducted by Thin Layer Chromatography (TLC), High-Performance Liquid Chromatography (HPLC), and Ultra High-Performance Liquid Chromatography (UHPLC). TLC results indicated no visible spots associated with amoxicillin in the milk sample. HPLC chromatogram indicated a peak at 3.610 mins with characteristic UV peaks at 276, 228, and 194 nm for the amoxicillin standard (AS). The pasteurized milk sample indicated a peak at 4.085 mins with a UV peak at 276 nm, indicating the necessity for further verification. UHPLC analysis using isocratic and gradient techniques indicated peaks for AS at 2.950 and 2.949 mins, respectively, but corresponding peaks were not detected in the pasteurized or raw milk samples. Our study confirmed that amoxicillin residues were either absent or below the detectable level in the pasteurized milk samples analyzed. As a result, the pasteurized milk samples were confirmed to be free of amoxicillin residues, ensuring compliance with safety regulations in Sri Lanka.

#### **Keywords:**

Antibiotic; Amoxicillin; Milk; HPLC; TLC.

### Acknowledgement:

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*Abstract No: 2025\_282* 

# Antioxidant and photoprotective properties of *Flacourtia indica* fruit extract: fractionation, and application in lipstick formulation

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Flacourtia indica, known as Ugurassa in Sri Lanka, is widely recognized for its ethnomedicinal applications. Despite its traditional use, scientific studies on its antioxidant and photoprotective properties remain limited. This study aimed to evaluate the antioxidant and photoprotective properties of F. indica fruit extract, perform sequential fractionation to identify bioactive fractions and incorporate a suitable bioactive fraction into a lipstick formulation to develop a herbal multifunctional lipstick. Chemical constituents in dried fruit powder were extracted by maceration using hexane, acetone, ethanol:water (80%v/v), and methanol. The highest extraction efficiency (12.13%) was obtained with ethanol:water (80%v/v). The total phenolic content (TPC) and total flavonoid content (TFC) in ethanol: water (80%v/v) extract were determined using Folin-Ciocalteu and aluminum chloride assays, respectively, yielding  $21.10 \pm 0.01$  mg GAE/g and 34.70± 2.20 mg CE/g. Antioxidant potential was assessed using 2,2-diphenyl-1-picrylhydrazyl (DPPH) radical scavenging (IC<sub>50</sub> = 782.94  $\pm$  12.61 µg/mL) and ferric reducing antioxidant power (FRAP) (0.348 ± 0.008 mg BHT/g) assays. The photoprotective property was evaluated by determining the sun protection factor (SPF) spectrophotometrically with the Mansur equation, which indicated moderate UV protection  $(17.19 \pm 1.63)$ . Sequential fractionation of the extract was performed using hexane, chloroform, ethyl acetate, and methanol. SPF evaluation showed notable values for the hexane (30.85  $\pm$  2.84), chloroform (17.19  $\pm$ 1.63), and methanol (15.99  $\pm$  0.65) fractions. The methanol fraction exhibited the highest antioxidant activity (DPPH, IC<sub>50</sub> = 296.50  $\pm$  2.27 µg/mL). As the methanolic fraction was red and exhibited antioxidant and photoprotective properties, it was incorporated into a lipstick formulation. The developed lipstick formulation was evaluated for color (dark red), texture (smooth), pH (5.6), melting point (53 °C), and skin compatibility (no skin irritation), confirming its suitability according to the Bureau of Indian Standards 9875:2018 guidelines for application, contingent upon the completion of toxicity studies.

## **Keywords:**

*Flacourtia indica*; Antioxidant; photoprotective properties; lipstick.

# Chitosan-Stabilized Silver Nanoparticles: Molecular Dynamics Simulation on the Stability and *in-vivo* Interactive Toxicity with Cadmium on an Aquatic Model *Moina macrocopa*

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Silver nanoparticles (AgNPs) are a significant innovation in nanoscience, particularly for their potential applications in biological systems. In this study, silver nanoparticles were synthesized using chitosan acting as both reducing and capping agent, characterized by UV-visible spectroscopy, and Transmission Electron Microscopy (TEM), Fourier-Transform Infrared Spectroscopy (FTIR), and X-Ray Diffraction (XRD). The surface plasmon resonance peak of CS-AgNPs was identified at 440 nm. TEM revealed spherical particles with an average of 12nm in size. XRD patterns confirmed crystalline silver with a face-centered cubic structure. Molecular docking revealed weak non-bonding interactions with a +0.03 kcal/mol binding energy. In a water simulation model, molecular dynamics simulations were performed to predict the stability of CS-AgNPs compared to bare AgNPs. Radius of gyration (Rg) and Root Mean Square Deviation (RMSD) indicated the stabilization of CS-AgNPs throughout the 50 ns simulation length. The toxicity of CS-AgNPs and their interactive effects with Cd were evaluated in-vivo using the freshwater zooplankton, Moina macrocopa (age <24 hours). Acute toxicity tests revealed a notable change in 24-hour LC<sub>50</sub> values upon exposure to AgNO<sub>3</sub>, CS-AgNPs, CdSO<sub>4</sub>, and combined (CS-AgNPs + Cd), which were 0.005,

0.056, 0.057, and 0.036 mg/L, respectively. Chronic toxicity tests revealed a significant reduction in body length, population size, and the total reproductive output of the exposed individuals to the chemical mixtures for 7 days (p < 0.05). Synergistic toxicity was observed in the combined exposure to both acute and chronic toxicity studies. In conclusion, CS-AgNPs demonstrated significantly reduced toxicity compared to their Ag+ counter concentrations, and molecular dynamics revealed the better stability of AgNPs when they were coated with chitosan, highlighting their applications in nanomedicine and industries. The interactive toxicity of CS-AgNPs with Cd metal ions on *M. macrocopa* highlights the need to optimize their safe concentrations for ecological safety.

# Keywords:

Silver nanoparticles, CS-AgNPs, *Moina macrocopa*, toxicity, molecular dynamics

# Acknowledgment:

This research is funded by the Department of Chemistry, University of Kelaniya & Department of Zoology and Environmental Management, University of Kelaniya

# Electrochemical Impedance Spectroscopy for Prediction of Corrosion Inhibition of CaO Nanoparticles toward Grade 202 Stainless-steel

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Grade 202 Stainless Steel (SS Grade 202) offers excellent corrosion resistant characteristics under mild conditions due to the presence of a relatively high chromium percentage although it is an alloy rich in iron. The impact of various chemical components that are present in the environment on its corrosion behavior, and the potential use of corrosion inhibitors under such situations, has not been extensively studied. Conversely, certain nanoparticles inhibit corrosion by adhering to metal surfaces, thereby creating a protective barrier that blocks the exposure to corrosive agents. NPs of CaO derived from clamshells serve as highly effective corrosion inhibitors due to their minuscule size and expansive surface area, which aid in the passivation of oxide films, including chromium oxide on SS. The abundant availability of clamshells makes them a sustainable source for producing CaO NPs. Application of electrochemical impedance spectroscopy (EIS) on SS Grade 202 in the presence of CaO NPs in acidic medium, with the aid of Nyquist and Bode plots, results in a notable increase in polarization resistance (RP) and total impedance, respectively, demonstrating the corrosion inhibitory behavior. In

particular, change in the concentration of CaO NPs from 1.00 mmol L<sup>-1</sup> to 5.00 mmol L<sup>-1</sup> in 4.00 mol L<sup>-1</sup> acetic acid enhances the extent of corrosion inhibition from 92.1% to 97.6%, as determined from RP values, whilst the change in the phase angle maxima from 50° to 80° demonstrates the formation of a strong passive film in the presence of CaO NPs. EIS provides evidence for corrosion inhibition of SS Grade 202 by CaO NPs in sodium acetate and ammonium acetate solutions as well. Moreover, an increase in the concentration of acetic acid and ammonium acetate enhances the rate of corrosion according to EIS and Bode plots. On the other hand, sodium acetate functions differently, performing as a corrosion inhibitor toward SS.

### Keywords:

Bode plots, CaO NPs, corrosion, inhibition, EIS

## Acknowledgments

Special appreciation for the immense support provided by the Department of Chemistry, Faculty of Science, University of Peradeniya, Sri Lanka.

# Formulation of *Psidium guajava* Linn essential oil encapsulated solid lipid nanoparticles and evaluation of its anti-inflammatory and antioxidant activity

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Essential oils (EOs) possess significant therapeutic properties but are limited by volatility, instability, and poor bioavailability. This study aimed to encapsulate Psidium guajava Linn EO within solid lipid nanoparticles (SLNPs) to enhance its stability and biological efficacy. The objectives were to extract EO from *P. guajava* leaves through hydrodistillation, encapsulate EO into SLNPs, characterize the nanoparticles, and evaluate their antioxidant and anti-inflammatory activities. SLNPs were prepared using high-shear homogenization followed by ultrasonication, utilizing cocoa butter (1.8 g) as the lipid matrix, lecithin (1.2 g) as the emulsifier, and distilled water (196 ml) as the aqueous phase. The EO-loaded SLNPs exhibited a particle size range of 139.7-145.9 nm with a polydispersity index below 0.3, indicating uniform size distribution. A highly negative zeta potential (-46.8 to -48.2 mV) confirmed good colloidal stability, reducing aggregation risks. Fouriertransform infrared spectroscopy (FTIR) confirmed successful encapsulation without chemical degradation, while scanning electron microscopy (SEM) revealed smooth, spherical to slightly elongated nanoparticles. Encapsulation efficiency was 77.94%, with a loading capacity of 20.65%, ensuring effective entrapment of EO

within the lipid matrix. Antioxidant activity, assessed *via* the DPPH assay, showed that free EO had an  $IC_{50}$ of 42.68 ± 2.01 mg/mL, whereas encapsulated EO had a slightly higher IC<sub>50</sub> of 56.81  $\pm$  2.14 mg/mL, indicating a controlled-release effect. Despite a minor reduction in radical scavenging activity, encapsulation significantly improved EO stability, reducing susceptibility to oxidation. Anti-inflammatory activity, evaluated using the egg albumin denaturation assay, demonstrated that EO-loaded SLNPs exhibited a higher inhibition (47.73  $\pm$  1.44%) than free EO (42.28  $\pm$  3.40%), suggesting enhanced bioavailability and prolonged therapeutic effects. Overall, nanoencapsulation improved the stability, controlled release, and therapeutic potential of *P. guajava* EO, making SLNPs a promising delivery system for pharmaceutical applications. Future studies should optimize formulation parameters and conduct in vivo studies for clinical validation.

### Keywords:

essentialoil, solid lipid nanoparticles, nanoencapsulation, antioxidant activity, anti-inflammatory activity.

# Investigation of catalytic properties of green synthesized copper oxide nanoparticles in Biginelli reaction

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Biginelli-type synthesis is an efficient one-pot synthesis method for preparation of 3,4-dihydroxypyrimidine derivatives, which have many pharmaceutical properties. Use of a Lewis acidic earth abundant transition metal oxide such as nano-copper oxide rather than concentrated HCl, as the catalyst, allows Biginelli reaction to be conducted in a greener approach. The catalytic potential of green synthesized copper oxide nanoparticles was studied in two Biginelli type reactions. Black tea leaf waste powder-aqueous extract (BTLE) was prepared by heating the tea waste powder (5 g) with double distilled water (100 ml) at 60 °C for two hours. Synthesis of copper oxide nanoparticles was done by mixing [Cu(CH<sub>2</sub>COO)<sub>2</sub>].H<sub>2</sub>O (2.795 g), dissolved in double distilled water (70 ml), with BTLE (20 ml). The calcination temperature was 320 °C. Based on the powder-XRD of the synthesized nanoparticles, the copper (I) oxide was majorly present with a lower fraction of copper (II) oxide. SEM image analysis revealed nanoparticle (50-100 nm) aggregates of few micrometers (1-5  $\mu$ m). To study the catalytic activity of the nanoparticles in the Biginelli reaction, the reaction between urea, ethyl acetoacetate, and benzaldehyde was conducted with variation of time from one, two, and eight hours with the reagent stoichiometry controlled

at 1.0: 1.1: 1.1 equivalents of benzaldehyde, ethyl acetoacetate, and urea, respectively, in refluxing ethanol. In each trial, a constant amount of copper oxide catalyst (30 mg) was used. The obtained crude was recrystallized with ethanol. When the reaction time was increased from one hour to two hours, the Biginelli product yield increased from 26.0 % to 29.0 %. At the end of eight hours, the Biginelli product was obtained at a 31.8 % yield. The <sup>1</sup>H NMR and the FTIR analysis confirmed the formation of the pure product, ethyl 6-methyl-2-oxo-4-phenyl-1,2,3,4-tetrahydropyrimidine-5-carboxylate. The reaction between urea, ethyl acetoacetate, and 4-methoxybenzaldehyde, conducted under the same reaction conditions for eight hours, yielded the methoxy derivative of Biginelli product in 8.7%. Formation of the product was confirmed by FTIR and <sup>1</sup>H NMR analysis. The lesser yields in the Biginelli type reactions indicate that green synthesized copper oxide nanoparticles with high copper (I) oxide content do not act as an efficient catalyst in Biginelli type reactions.

#### Key words:

Green synthesis, Copper (I) oxide, catalysis, Biginelli reactions

# Evaluation of *Justicia adhatoda* Linn. extract-loaded layered double hydroxide nanohybrid for sunscreen applications

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Safety concerns regarding synthetic sunscreens have increased the demand for botanical alternatives rich in phytochemicals with natural photo-protectant properties. Layered double hydroxides (LDHs) offer biocompatibility, tunable composition, high anionexchange capacity, and controlled release. This study focused on developing a plant extract-incorporated LDH nanohybrid and evaluating its photostability and antioxidant activity. Based on the UV blocking ability at UVA and UVB regions, J. adhatoda was selected. The sun protection factor (SPF) of ethanolic J. adhatoda leaf extract was evaluated using UV spectroscopy and the Mansur equation. Pristine MgAl-NO<sub>3</sub>-LDH was synthesized via co-precipitation with a Mg: Al ratio of 2:1, adjusting the pH to 10 using 1.0 M NaOH. J. adhatoda-LDH (JA-LDH) nanohybrid was prepared via ion exchange by adding pristine MgAl-NO<sub>3</sub>-LDH (1.500 g) suspension to J. adhatoda crude extract (2.000 g) dissolved in DMSO (50 mL). Pristine MgAl-NO<sub>2</sub>-LDH and JA-LDH were characterized using FTIR, XRD, and SEM imaging. The antioxidant activity of J. adhatoda crude extract and JA-LDH was evaluated by

the DPPH radical scavenging assay. The photostability of J. adhatoda crude extract and JA-LDH hybrid was assessed by exposing them to direct sunlight for 3 hours. The SPF value of ethanolic J. adhatoda leaf extract was 8.16 at 250 ppm, and with increasing concentration, the SPF value increased. FTIR of JA-LDH showed characteristic bands of pristine MgAl-NO<sub>3</sub>-LDH and J. adhatoda extract, confirming successful incorporation. XRD revealed a change in basal spacing from 8.508 Å to 7.679 Å upon incorporation, and SEM images showed morphological changes supporting incorporation. The percentage incorporation efficiency of J. adhatoda leaf extract in pristine MgAl-NO<sub>3</sub>-LDH was 13.0%. The IC<sub>50</sub> value of *J. adhatoda* was 15.64 µg/mL, while the IC<sub>50</sub> value of JA-LDH was 13.01 µg/mL. JA-LDH showed photostability, indicating LDH stabilizes the incorporated phytochemicals. It is concluded that the JA-LDH is suitable for developing novel sunscreens.

# Keywords:

Layered double hydroxide; *Justicia adhatoda* Linn.; Antioxidant; Sun protection factor; Photostability.

# Use of Aqueous Na<sub>2</sub>CO<sub>3</sub> Systems for Inhibition of Corrosion of Grade 202 Stainless-steel

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Corrosion is a process that promotes damaging attack on a metal by chemical or electrochemical reaction with the environment it is exposed to. Corrosion has been driven its concern due to costly maintenance, and hence, inhibitors are needed to avoid this undesirable situation. Inhibitors slow down the corrosion rate through various means, out of which the formation of a passive film is common. Although stainless steel (SS) has corrosion risk in aggressive environments, it is known for its strong corrosion resistance in mild environments comparative to other alloys, mainly due to the presence of chromium which forms a barrier of its oxide. To improve the life-time of SS, sustainable corrosion inhibitors with cost-effective constituents have been employed. However, detailed investigation of the reactivity of various dissolved salts on the corrosion inhibition action of Grade 202 SS has not been much elaborated. This study is thus focused on a multitechnique approach to investigate the effect of acidic conditions on the corrosion inhibition of aqueous Na<sub>2</sub>CO<sub>3</sub> systems. Mass loss measurements indicate that 0.25 mol L<sup>-1</sup> Na<sub>2</sub>CO<sub>3</sub> acts as a corrosion inhibitor with the inhibition efficiency of 99.82% in the presence

of 0.25 mol L<sup>-1</sup> HCl, which was further increased when the concentration of  $Na_2CO_3$  is increased, achieving a superior corrosion inhibition efficiency. Electrochemical impedance spectroscopy indicates that the polarization resistance, which is inversely related to the corrosion rate, increases with the increase in the concentration of  $Na_2CO_3$  at the fixed concentration of HCl, supporting mass loss measurements. Moreover, open circuit potentials of Grade 202 SS are increased when the concentration of  $Na_2CO_3$  is increased, further supporting. Comparison of the corrosion inhibitory action of  $Na_2CO_3$  in the presence of HCl, HNO<sub>3</sub>, and CH<sub>3</sub>COOH indicates that the extent of inhibition follows the order, HCl < HNO<sub>3</sub> < CH<sub>3</sub>COOH.

## Keywords:

Corrosion, impedance, inhibition, mass loss measurements, Na<sub>2</sub>CO<sub>3</sub>

### Acknowledgement

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# α-Amylase Inhibitory Activity of Fractions Separated from The Seed Extract of Syzygium cumini (L.) Skeels

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Diabetes mellitus (DM) ranks a world-wide metabolic disorder in which chronic hyperglycemia arises due to insulin dysfunction. Syzygium cumini, a plant with medicinal properties and a tradition of being used for diabetes in Sri Lanka, was then confirmed to have antidiabetic potential. This study aims to isolate, and separate bioactive compounds from the seed ethanolic extract of Syzygium cumini (L.) Skeels and to evaluate their potential  $\alpha$ -amylase inhibitory activity. Seeds of Syzygium cumini Skeels were extracted to ethanol by sonication at 40 °C for 2 hours. Then the extract was subjected to chromatographic separation using silica gel (230-400 mesh) as the stationary phase. Gradient elution was carried out using 30 ml of hexane:ethylacetate solvent system in ratios of (9:1), (8:2), (7:3), (6:4), (5:5), (4:6), (3:7), (2:8), and (1:9). Each fraction was analyzed by thin layer chromatography (TLC) and fractions with similar TLC profiles were combined. Spot visualization of TLC was done under a 365 nm UV lamp, and according to the TLC results, six individual spots were identified. Six isolated fractions were further purified using the preparative TLC method.

The bioactivities of isolates were assessed through invitro a-amylase bioassay, each at a concentration of 1 mg/ml. Six isolates showed significant α-amylase inhibitory activity, out of which two have shown inhibition percentage (88.45% and 87.54%) comparable to that of a standard drug acarbose (91.83%). These findings suggest that these bioactive constituents may be responsible for the antidiabetic potential of S. cumini and thus should receive further investigation for any potential therapeutic use. This research highlights the significance of medicinal plants as a source of natural enzyme inhibitors, thereby providing a foundation for the development of plant-based antidiabetic agents. Further studies should focus on further purification, on structural elucidation, mechanism of action studies, and in-vivo validation of these bioactive compounds to facilitate their potential pharmaceutical application.

### Keywords:

Diabetes mellitus, *Syzygium cumini*, column chromatography, *in-vitro* α-amylase bioassay

# Antifungal efficacy of metallic silica nanohybrids embedded in hydrogel formulations for enhanced dermatological applications

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Fungal skin infections pose a significant and escalating global health threat, emphasizing the need for innovative therapeutic approaches. The incorporation of metallic silica nanohybrids into polymeric hydrogel formulations presents a promising strategy to address these infections. In this study, we synthesized a nanohybrid by doping silver (Ag), copper (Cu), and cobalt (Co) separately into silica nanoparticles using the sol-gel method, followed by mechanochemical grinding to combine the metals in equal proportions. The resulting nanohybrids were incorporated into a hydrogel matrix made from a 2% (w/v) solution of sodium alginate and carboxymethyl cellulose. Gel formulations were prepared at concentrations of 2, 3, 4, 5, 10, and 15 mg/mL by dissolving the nanohybrid dispersions in the polymer blend, followed by crosslinking with 2M calcium chloride solution (20% (v/v)). Characterization of the gel formulations included Fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), Raman spectroscopy, and scanning electron microscopy (SEM) for structural and morphological analysis. Atomic absorption spectroscopy (AAS) quantified the loading capacity

of metal in each formulation. The band gap energy of the gels was measured and recorded at around 2.94 eV using UV diffuse reflectance spectroscopy, confirming the potential for radical scavenging under visible light. Swelling index and porosity measurements indicated that the 15 mg/mL gel formulation exhibited the highest values, with a swelling index of 717.10±19.35% and porosity of 129.46±2.23%. Antifungal activity was evaluated using the agar overlay method, followed by colony count assays against Candida albicans, Trichophyton rubrum, Microsporum gypsum, and Epidermophyton floccosum. The 15 mg/mL formulation showed complete inhibition, with zero colony counts against all tested fungal strains. These findings underscore the promising potential of metallic silica nanohybrid-integrated hydrogel formulations as a highly effective and innovative therapeutic approach for treating dermatophytic and other fungal skin infections.

## **Keywords:**

Antifungal activity, Metallic, Nanohybrids, Hydrogel, Band gap energy

# Enhanced antimicrobial and anti-inflammatory properties of PCL metal-turmeric oleoresin and metal-curcumin nanohybrids

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The concern about microbial infections and antimicrobial resistance has now shifted towards designing sustainable biomaterials with greater therapeutic efficacy for hospitals and several biomedical applications, which involve the use of modern multifunctional nanomaterials that are currently being studied. This blend is incorporated into an electrospun mat of biodegradable polycaprolactone (PCL). This developed antimicrobial electrospun PCL membrane by incorporating curcuminoids and trimetallic nanoparticles (Ag, Cu, Ni), exhibited strong antibacterial, anti-inflammatory, and antioxidant activity against a range of microorganisms. The nanohybrids were synthesized and characterized using Fourier-transform infrared spectroscopy (FTIR), Raman spectroscopy, X-ray diffraction (XRD), scanning electron microscope (SEM), and UV diffuse reflectance spectrometry. The synergistic antimicrobial effect of the electrospun membranes containing a curcuminoid coupled trimetallic nanohybrid was demonstrated by the inhibition zones from 29.67 $\pm$  0.24 to 33.17  $\pm$  0.24 mm against several strains of bacteria and fungi. The evidence for the primary antibacterial action is the radical scavenging activity (RSA) that reached a high value of 76.14  $\pm$  0.99% in the PCL mat with trimetallic and curcuminoid incorporated nanohybrid. Moreover, curcuminoids showed impressive anti-inflammatory effects, with a peak value of 72.81  $\pm$  0.33% reduction at 5000 ppm. The electrospun membranes have

strong inhibiting activity against microbial growth and are non-toxic, environmentally friendly, and biodegradable. These membranes play a role in acting as a physical and biological barrier, a cost-effective, and environmentally safe substitute for conventional antimicrobial techniques. This research shows that trimetallic-curcuminoid nanohybrid electrospun membranes are viable as sustainable biomaterials for next-generation antimicrobial therapies that make biomedical applications safer and more effective while being environmentally friendly and biocompatible. It serves as an example of how creative approaches can address issues related to sustainability and health.

# Keywords:

Antimicrobial; Anti-inflammatory; Electrospun membranes; Metal- turmeric oleoresin; Metalcurcuminoids.

# Acknowledgment:

Financial support for this study is acknowledged by the University of Sri Jayewardenepura, Sri Lanka under the research grant number ASP/ 01/ RE/ SCI/ 2022/15 and The World Academy of Science (20/102/ RG/ CHE/ AS\_1 - FR3240314134) for providing grants for the electrospinning setup. Authors acknowledge the Instrument Centre, Faculty of Applied Sciences, University of Sri Jayewardenepura for the facility provided in analysis and characterization.

# Harnessing the Power of Visible Light with GO-Ni-ZnO Nanohybrid Electrospun Polymeric Membranes for Improved Photocatalysis: A Focused Approach to Fabrication, Characterization, and Applications

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Photocatalysis exhibits considerable potential for a range of environmental, energy, and biomedical applications, especially when employing metal-doped nanoparticle systems like Ni-doped ZnO. By giving nanohybrid stability and structural support, graphene oxide (GO) enhances photocatalytic activities and increases its durability and resistance to photocorrosion. Electrospinning is used to create GO-Ni-ZnO nanohybrid membranes, which are then characterized by FTIR, Raman spectroscopy, SEM, XRD, and UV diffuse reflectance spectroscopy. The outcomes show a notable improvement in the organic dye methylene blue's photocatalytic breakdown when exposed to visible light, underscoring the membranes' environmental remediation and potential for wastewater treatment. After 15 minutes, a nanohybrid consisting of 4% graphene oxide (GO) and 5% nickeldoped zinc oxide (Ni-doped ZnO) incorporated into a cellulose acetate electrospun mat produced the greatest photocatalytic activity of 93.41%. This outcome validates the nanohybrid system's synergistic benefits. The DPPH assay was used to measure radical scavenging activity (RSA), which is thought to be the main mechanism underlying this occurrence. With a rate constant of 0.3208 mM/min for the nanoparticles, the nanohybrid mat showed the highest RSA, achieving 80.44% of radical scavenging activity after 60 minutes. This electrospun mat's gap energy, which

was measured at 3.1346 eV, provides more evidence of the nanohybrid system's efficacy in visible light. Furthermore, an antimicrobial test demonstrated the mat's potent antibacterial qualities, showing the biggest zones of inhibition (between 25.5 and 33.0 mm) against pathogens like Salmonella typhi, Shigella sonnei, Candida albicans, Escherichia coli, and Staphylococcus aureus. All things considered, GO-Ni-ZnO nanohybrid electrospun membranes offer a viable strategy for raising photocatalytic efficiency, providing affordable and environmentally friendly answers for a range of uses.

# Keywords:

Photocatalysis; Dye degradation; Semiconductor; Electrospinning; Antimicrobial.

# Acknowledgment:

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# Copper-zinc oxide nanohybrids for advanced antimicrobial and photocatalytic applications

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ZnO exhibits remarkable photocatalytic and antimicrobial activity as a nanomaterial for diverse applications, including environmental remediation, healthcare, and sustainable energy solutions. However, a major problem with ZnO photocatalyst is that it is active only under UV irradiation owing to its high band gap. Doping transition metals like Cu into the ZnO lattice offers an effective solution to addressing the limitations of pure ZnO, especially lowering the band gap energy. In this research examines the enhanced photocatalytic sterilizing effectiveness of Cu-doped ZnO nanoparticles that are active in visible light. Using the co-precipitation method, Cu-ZnO nanohybrids (CuxZn100-xO) have been generated using a range of dopant ratios (x = 0, 3, 5, 7, and 10) at different calcination temperatures of 450 °C and 650 °C to compare their activities. They were characterized structurally by Fourier transform infrared (FTIR), Raman spectroscopy, and X-ray diffraction (XRD). Band gaps of nanohybrids were characterized by Ultraviolet-Visible diffuse reflectance spectroscopy (UV-Vis DRS). Scanning electron microscopy (SEM) images were used to characterize the morphology. The doped percentages of Cu into ZnO network were determined using atomic absorption

spectroscopy (AAS). The Cu 7%-ZnO synthesized at 450 °C nanohybrid, which has the lowest band gap (3.09 eV), exhibited the highest photocatalytic activity against Methylene blue under visible light. Moreover, the Cu 7%-ZnO exhibited the lowest IC50 value of 151 µg/ml compared to pure ZnO, indicating the highest radical scavenging activity. The highest inhibition zones were also shown by the Cu 7%-ZnO against the grampositive bacteria; *S. aureus*, gram-negative bacteria *E. coli*, S. *somnei*, *S. typhi*, and fungi; *C. albicans*, while showing its synergistic antimicrobial activity. In conclusion, the Cu 7%-ZnO exhibits enhanced photocatalytic and antimicrobial properties, making it a promising candidate for applications in environmental and healthcare fields.

## Key words:

Zinc oxide, Copper, Photocatalytic activity, Antimicrobial activity, Band gap energy

## Acknowledgment:

Financial support for this study is acknowledged by the Institute of Chemistry Ceylon, Sri Lanka undergraduate research grant.

# Antioxidant Activity, Phytochemical Screening and GC-MS Profiling of Some Tea Varieties of Sri Lanka

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Tea is a widely consumed beverage made from the Camellia sinensis plant. The antioxidant properties of tea leaf extract have been extensively studied. The study aimed to analyse 19 commercially available tea varieties belonging to four groups, i.e., black, green, organic, and herbal tea, to identify key bioactive compounds. Methanol and dichloromethane were used as the solvents for extraction and the antioxidant activity was assessed using the DPPH (1,1-diphenyl-2-picrylhydrazyl) free radical scavenging assay using a UV-visible spectrophotometer measuring at a 517 nm wavelength to determine their efficacy in neutralizing free radicals. The phytochemical profile of the methanolic extract of the tea varieties was obtained by Gas Chromatography - Mass Spectrometry (GC-MS) analysis. Six samples of the 19 tea varieties analysed demonstrated superior antioxidant activity in the DPPH free radical scavenging assay. The tea variety with the best antioxidant activity was 26-KRT at 85.39%, followed by 21-BGT at 63.54%, 9-GTGPP at 61.15%, 3-LGTC at 59.71%, 7-OGT at 57.73%, and 6-PGT at 56.24%, with ascorbic acid serving as the

positive control (62.26%). The GC-MS analysis of the tea varieties identified several bioactive compounds, including 1,2,3-benzenetriol, 1-pentadecene, hexanoic acid, n-hexadecenoic acid, 9,12,15-octadecatrienoic acid methyl ester (Z,Z,Z)-, phytol, 9,12,15-octadecatrienoic acid (Z,Z,Z)-, 9,12-octadecadienoic acid (Z,Z)-, and theobromine. Caffeine was the main constituent among the compounds identified by GC-MS in all tea varieties except in herbal tea types such as Weniwelgata tea, Slim Apple tea, Mature tea, Pure Camomile tea, and DETOX. Phytochemical screening tests revealed the tea samples' abundance of alkaloids, flavonoids, polyphenols, saponins, and terpenes. These findings highlight tea extracts' effectiveness in preventing lipid oxidation during storage and their high antioxidant capacity, which provides additional health benefits and improves quality of life.

#### Keywords:

Camellia sinensis; GC-MS; antioxidants; Caffeine.

# Electrochemical Investigation of Thiamethoxam on Glassy Carbon Electrode

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Thiamethoxam (TMX) is one of the most widely used neonicotinoid pesticides in modern agriculture due to its unique properties, such as low toxicity to nontarget animals, including humans and mammals, with high target specificity; a broad spectrum of insecticidal action; and versatility in application methods. However, its persistence and water solubility contribute environmental contamination and potential to health risks, requiring sensitive detection methods. Electrochemical methodologies, due to their costeffectiveness and efficiency, offer a promising alternative to traditional techniques such as high-performance liquid chromatography and gas chromatography, which are tedious and costly and require specially trained personnel for operation. This study investigates the electrochemical behavior of TMX on a glassy carbon electrode (GCE) as a foundation for developing such electrochemical methodology. Cyclic voltammetry (CV) and square wave voltammetry (SWV) were used to characterize the reduction of TMX in various buffer solutions. The results revealed an irreversible reduction peak at -1.24 V, attributed to the reduction of the nitro group of TMX, occurring via a diffusioncontrolled process in pH 9.0 Britton-Robinson buffer (BRB) according to the peak current-scan rate relationship. More importantly, SWV demonstrated higher sensitivity than CV for the detection of TMX. Square wave voltammograms obtained at different pH values suggested that the maximum current was generated in pH 9.0 BRB. Although amperometric studies demonstrated the detection of TMX at the bare GCE, electrode fouling was observed as the large pesticide molecules interfere with the active surface for electrochemical reactions, suggesting the necessity of surface modification for improved analytical performance. This research establishes the feasibility of electrochemical methods for TMX detection and proposes the necessity of electrode surface modification to mitigate electrode fouling and enhance sensitivity.

## Keywords:

Amperometry, Cyclic voltammetry, Electrochemistry, Glassy carbon electrode, Thiamethoxam.

# Acknowledgments:

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# Synthesis of Cellulose Nanoparticles from *Panicum maximum* and their Application in Gas Filtration

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Air pollution is a significant global environmental issue. Excessive levels of oxides of carbon, nitrogen, and sulfur oxides cause a wide range of environmental complications, leading to various health problems. Environmentally friendly, economical, and sustainable approaches are essential to treat polluted air. Among various air filtering methods, such as electrostatic precipitation and chemical filtration, mechanical filtration and adsorption are more popular due to their low cost. Air filters made of synthetic polymers are non-biodegradable. The development of affordable membranes and adsorption materials for air filtering contributes to creating efficient devices to meet current and future global demand. This study aims to establish a green synthesis process for producing cellulose nanoparticles from the invasive and abundant weed Panicum maximum, which has no commercial value, to develop a gas-filtering device based on the membrane filtration technique. Cellulose nanoparticles possess high surface area, mechanical strength, and biodegradability. The dry grass sample was mechanically ground into fine powder (<63 µm), followed by delignification and bleaching to extract cellulose. The sample was de-lignified using NaOH, and it was neutralized through multiple washing steps. Subsequently, the sample was bleached with

NaClO, resulting in highly purified cellulose compared to the unbleached sample, as confirmed by Fourier Transformed Infrared Spectroscopy (FTIR) analysis. The purified cellulose was then hydrolyzed with formic acid to produce cellulose nanoparticles. These particles were analyzed using a granulometer, and it was revealed that the nanoparticles ranged in size from 4-170 nm. Scanning electron microscope (SEM) analysis revealed that the synthesized particles appeared in aggregated nature with particle size around 100 nm. To perform gas filtration using synthesized cellulose nanoparticles, cotton fabrics coated with these nanoparticles were tested for CO<sub>2</sub> filtration using a home-built setup. Preliminary experiments revealed a 90 ppm reduction in CO<sub>2</sub> concentration. Filtration optimization is currently being conducted by our group.

# Keywords:

Panicum maximum, cellulose nanoparticles, gas filtration

## Acknowledgment:

Special gratitude for the immense support provided by the Department of Chemistry, Faculty of Science, University of Peradeniya, Sri Lanka.

# Enhanced Removal of Ni(II) from Contaminated Solutions by NaOH-modified Tea Waste

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Heavy metal contamination is a critical environmental issue, requiring efficient and low-cost removal techniques. Among various types of removal techniques, adsorption has achieved much consideration due to different aspects. The heavy metal Ni is one of the major toxic heavy metals, which is primarily released from the combustion of fossil fuel and can accumulate across different organisms, leading to severe health disorders. Use of biosorbents in raw and modified forms for the remediation of Ni has been attempted; however, the removal efficiency has not been satisfactory, partly due to the lack of the number of active adsorption sites. The study reported here is on the investigation of tea waste (particle size: 0.500 -0.710 mm) modified with 0.10 mol L<sup>-1</sup> NaOH solution for enhanced removal of Ni(II) through biosorption. Variation of one experimental parameter within a reasonable range while keeping the other parameters unchanged lead to the optimized conditions of 0.600 g dosage, 20 min shaking time, 20 min settling time and ambient pH and at ambient temperature, at which an excellent removal of 95% is achieved from 10 mg L<sup>-1</sup> Ni(II) solution, based on the average values of triplicate measurements. This is a significant improvement when

compared to unmodified biosorbent which shows only 69% removal. Further, NaOH treatment would form negatively charged functionalities leading to complexation with the positively charged adsorbate, Ni<sup>2+</sup>. Since the Ni(II)–NaOH modified tea waste system establishes equilibrium so fast that it is not possible to investigate kinetics, further supporting the superior nature for biosorption of Ni(II). Increase in the initial concentration of Ni(II) from 10 mg L<sup>-1</sup> to 25 mg L<sup>-1</sup> does not significantly increase the time required to reach equilibrium, indicating that NaOH-modified tea waste is a promising biosorbent having strong capacity to remove Ni(II) from contaminated solutions within a short period of time.

# Keywords:

Adsorption, dosage, Ni<sup>2+</sup> remediation, shaking time, tea waste

### Acknowledgments:

Special appreciation for the immense support provided by the Department of Chemistry, Faculty of Science, University of Peradeniya, Sri Lanka.

# Quantitative analysis of morphology of microplastics in small pelagic fish species from the western and north-western coastal waters of Sri Lanka

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Microplastics (MPs) are a significant environmental issue, and particularly, coastal regions of countries like Sri Lanka with dense coastal populations and poor waste management are the hotspots of microplastics. Thus, the aims of this study are to quantify the MPs ingestion by small pelagic fish species from coastal fisheries and to assess whether there is any significant difference in the MPs pollution levels of fish in different locations of coastal waters from Kalpitiya to Negombo. A total of 109 individuals belonging to three species (Decapterus spp., Sardinella spp., Hirundichthys spp.) caught from one-day boats were collected from Kalpitiya, Chilaw, Thoduwawa, Wennappuwa, and Negombo fishery harbors during March to September of 2024. The fish were analyzed for MPs in their gills and gastrointestinal tracts using an alkaline digestion method (15% KOH), followed by microscopic examination. The MPs were categorized by color, shape, and size. In total, 149 MPs were found across all fish species. Hirundichthys spp. had the highest MPs ingestion (1.8 items individual<sup>-1</sup>), followed by Sardinella spp. (1.6 items individual<sup>-1</sup>) and Decapterus spp. (1.6 items individual<sup>-1</sup>). There was no significant difference in MP contamination between the species. When comparing MP levels by location, Decapterus spp. showed the highest MP abundance

in Wennappuwa (3.3 items individual<sup>-1</sup>), followed by Thoduwawa, Negombo, and Chilaw. *Sardinella* spp. also had the highest MPs in Wennappuwa and the lowest in Kalpitiya, while *Hirundichthys* spp. showed similar contamination levels between Chilaw and Negombo. There were no statistically significant differences between locations and MP contamination. In *Hirundichthys* spp. (32%) and *Sardinella* spp. (39%), most MPs measured 1000–5000 µm. *Decapterus* spp. showed 38% of MPs <250 µm. Blue (63%) and filamentous (70%) MPs dominated across all species. The findings highlight the impact of MP pollution on marine life, particularly in Wennappuwa, stressing the need for better waste management.

### Keywords:

Microplastics, Small Pelagic Fish, Coastal Waters, Sri Lanka

#### Acknowledgement:

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# A study of microplastics present in edible salts in Sri Lanka

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Microplastics (MP) are defined as plastics with a size less than 5 mm. Plastic debris, the origin of MP, has become a significant environmental pollutant. MP can cause more severe diseases in the respiratory, digestive and circulatory systems. The objective of this study was to investigate the presence of MP in commercially available crystalline and table salt in Sri Lanka. One brand of crystalline salt and six brands of table salt were selected with manufacturing date ranging from 2023 November to 2024 April. Precautionary measures were taken to minimize possible contamination with plastics from external sources. Blank experiments were carried out. A known quantity of salt samples was oxidized using H<sub>2</sub>O<sub>2</sub> to eliminate any organic matter present. MP were isolated by filtering and stained by acid red-1 dye. Color, shape and abundance were studied using a light microscope. Polymer types were identified by ATR-FTIR spectroscopy and Open Specy software. Morphology was studied using Scanning Electron Microscope. All the analyzed salt samples were contaminated with MP with an average concentration of 314 particles/kg. Average concentrations of MP in crystalline and table salt were 222 particles/kg

and 335 particles/kg, respectively. The morphologies determined for isolated MP included fibers (49 %), fragments (17%), pellets (23%), and spherical particles (12 %). When considering the color, transparent (199 particles/kg) was the predominant type of MP followed by black, brown, blue, red and green. Nine types of polymers were observed. Polyethylene was the most abundant (23%) polymer. Other polymers found were polypropylene, polyvinyl chloride, polyethylene terephthalate, acrylonitrile, cellulose nitrate, nylon, chlorinated polyethylene and acrylonitrile styrene. The findings underscore the urgent issue of MP contamination in salt, which poses significant health risks and threatens ecosystem conservation. Immediate measures such as sustainable development practices incorporating green chemistry are necessary to mitigate MP contamination, emphasizing that economic growth should not compromise sensitive ecosystems.

# Keywords:

Microplastics; table salt; crystalline salt; polymer; Sri Lanka

# Interpretation of Cr(III) adsorption by water hyacinth (*Eichhornia crassipes*) biosorbent through kinetics and isotherm analysis

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Water contamination by chromium species is a serious environmental and health issue, making its removal from water sources a top priority. Adsorption is a wellestablished method for heavy metal removal, with biosorbents emerging as an eco-friendly and costeffective alternative to synthetic adsorbents. In this study, water hyacinth (WH) powder extracted from live plants was explored as a natural biosorbent for removing Cr(III) from synthetic contaminated water. The dried WH powder (300–500  $\mu$ m) under optimum conditions of solution pH, dosage, shaking time and settling time achieves an impressive extent of removal of 95%. Fourier transform infrared spectroscopic analysis identifies -OH, C-O-C and C=O functional groups present in the biosorbent which would aid in complexation with Cr(III), which is supported by shifts in band positions upon interaction with Cr(III) solution. X-ray fluorescence spectroscopy confirms the uptake of chromium with an additional peak

appearing for Cr, while scanning electron microscopic images reveal structural changes on the surface after adsorption of Cr(III) from solution. The point of zero charge determined at pH = 8 indicates that the biosorbent functions well under slightly alkaline conditions. At equilibrium, the adsorption behavior aligns the best with the Sips adsorption isotherm, combining characteristics of both the Langmuir and the Freundlich isotherm models, indicating a combination of monolayer and multilayer adsorption. These findings demonstrate that WH powder is a highly efficient and sustainable biosorbent for Cr(III) removal, offering a low-cost and environmentally friendly solution for water purification.

# Keywords:

Adsorption; biosorbent; *Eichhornia crassipes*; isotherm; point of zero charge

# Altering bioavailability in curcumin derivatives- an *in silico* study

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Curcumin and its derivatives exhibit diverse pharmacological activities, including antioxidant, anti-inflammatory, anti-proliferative, antibacterial, analgesic, and antiviral effects. However, their therapeutic potential is often limited by poor bioavailability, primarily due to low intestinal absorption. In this in silico study, we screened 198 curcumin derivatives identified in previous studies for toxicological profiles, bioavailability, and drug-likeness. Structural similarities among the derivatives were analyzed using Tanimoto similarity indices to identify key structural features influencing pharmacokinetic properties. This structural analysis was used to identify trends that could be attributed to receptor binding and guide the development of novel curcumin derivatives with improved drug-like properties. The top-ranked molecules from the screening were geometry optimized via Gaussian with a basis set of 6-311G++dp using the B3LYP hybrid density functional theory. The resulting molecules were then subjected to molecular docking (using Autodock Vina) against the human intestinal oligopeptide transporter 1 (PepT1), a known active transporter involved in drug absorption. Among the tested derivatives, the molecule designated as "C09"

exhibited the highest docking score of -8.5 kcal mol<sup>-1</sup>, suggesting strong binding affinity to PepT1. To further enhance bioavailability, the same set of curcumin derivatives was conjugated with a dipeptide and reassessed for binding interactions with PepT1. The results indicated that dipeptide-conjugated curcumin derivatives consistently displayed higher docking scores compared to their non-conjugated counterparts. The enhanced binding affinities of dipeptide-conjugated derivatives were attributed to additional stabilizing interactions with key residues in the PepT1 binding pocket, including LYS140, ARG27, ASN171, TYR31, GLU595, and TRP294. These findings suggest that dipeptide conjugation enhances the interactions of curcumin derivative with PepT1, potentially improving absorption and bioavailability. This study provides a rational basis for designing bioavailable curcumin derivatives and highlights the role of structural similarity analysis in optimizing drug candidates.

# Keywords:

Curcumin derivatives; drug-likeness, intestinal absorption; PepT1; molecular docking

# Exploring bioactive compounds and antioxidant activity of selected Sri Lankan medicinal plants for skincare innovation

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Skin cancer, premature aging, and wrinkle formation are major global health concerns caused by prolonged exposure to UV radiation. There is an emerging trend for applying natural plant extracts as a solution of antioxidants and other bio-active compounds. Seeds and leaves of 17 medicinal plants used in Sri Lankan traditional healing practices were extracted with a 1:1 (v/v) methanol-dichloromethane solvent at a 1:5 (w/v)plant-to-solvent ratio. The extracts were screened for phytochemicals, identified by GC-MS, and assessed for antioxidant activity using DPPH (2,2-diphenyl-1-picrylhydrazyl). The phytochemical screening confirmed the presence of flavonoids, alkaloids, phenols, tannins, terpenoids, saponins, carbohydrates, sterols and triterpenes in plant extracts. Among the 17 tested plants, those with the highest antioxidant activity included the leaves and fruits of Elaeocarpus serratus (Ceylon Olive), Psidium guajava (Guava), Punica granatum (Pomegranate), Psidium cattleyanum (Cherry Guava), leaves of Flueggea leucopyrus (Katupila), fruits of Ixora coccinea (Rathmal) and seeds of Dialium ovoideum (Tamarind velvet). GC-MS analysis revealed key antioxidant compounds with significant peaks, including trans-4-methoxychalcone and 2H-pyran2,6(3H)-dione in E. serratus leaves and fruits, humulene and methyl 10-trans,12-cis-octadecadienoate in P. guajava leaves and fruits, (2R,3S,4S,5R)-2,5-bis(3,4dimethoxyphenyl)-3,4-dimethyltetrahydrofuran in P. granatum leaves, caryophyllene oxide and 9-oxabicyclo[6.1.0]non-6-en-2-one in P. cattleyanum leaves and fruits, 1-methyl-1H-Pyrrole in F. leucopyrus leaves, 2-oxo-butanoic acid in I. coccinea fruits, and scyllo-inositol in D. ovoideum seeds. The fruit of E. serratus exhibited the highest significant antioxidant activity (73.8%, p < 0.05), followed by its leaves (54.8%). In contrast, the lowest activity was observed in D. ovoideum seeds (3.6%) compared to 200 ppm ascorbic acid (standard) showed 62.26%. The results of the current study identify the fruit and leaf extracts of E. serratus as a promising source for pharmaceutical products aimed at addressing skin cell damage and preventing skin cancer. Further studies will evaluate their anti-cancer potential, advancing the development of nature-based skincare formulations.

#### Keywords:

GC-MS; Antioxidant; Phytochemicals; E. serratus

# Assessment of microplastic pollution in water and sediment: a preliminary study in Uma-oya and Badulu-oya sub-catchments of the Mahaweli river, Sri Lanka

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Microplastics ( $\leq 5$  mm) are emerging global pollutants. Their accumulation in freshwater ecosystems converts these into contaminant sinks, making microplastic pollution a significant global issue. While numerous studies have examined microplastics in marine ecosystems, research on microplastic pollution in Sri Lankan rivers remains limited. Hence, this study investigated the presence of MPs in the Uma-Oya (UO) and Badulu-Oya (BO) sub-catchments of the Mahaweli River. In June 2024, water and sediment samples were collected from ten sites, with a total of 20 surface water samples (n=20) and 30 sediment samples (n=30)analyzed. MPs in sediments were extracted using density separation and organic matter digestion, while surface water residues (0.125-5 mm) underwent KOH digestion and density separation with NaCl. Filtered samples were analyzed using a stereomicroscope, and ATR-FTIR identified polymer types in particles larger than 5 mm. Microplastics (MPs) in the sediments of Uma Oya and Badulu Oya were found in various colors, with blue being the most dominant, accounting for 35.14% and 35.53%, respectively. Similarly, in surface water, blue MPs were the most prevalent, making up 29.25% and 27.37%, respectively. Fibershaped MPs were the most abundant in sediments (UO; 67.56%, BO; 76.32%) and surface water (UO;

53.06%, BO; 50.43%). The most common MP size in sediments was 1–2.5 mm (UO; 43.24%, BO; 40.79%), while in surface water, it ranged from 1–2.5 mm (UO; 38.1%, BO; 36.49%). The mean MP abundance in surface water was  $1.05 \pm 0.095$  and  $2.67 \pm 1.51$  items/m<sup>3</sup>, while in sediments, it was  $9.99 \pm 5.39$  and  $12.49 \pm 11.02$  items/kg. ATR-FTIR identified polypropylene, high-density polyethylene, styrene ethylene butylene styrene, polyethylene terephthalate and polypropylene copolymer as polymer types. This study demonstrates the widespread presence of microplastics in Uma Oya and Badulu Oya, highlighting their significant contribution to freshwater pollution and underscoring the need for targeted pollution management strategies.

# Keywords:

Badulu oya; freshwater; microplastics; sediment; Uma oya

### Acknowledgement:

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# Microplastics in Sri Lankan freshwater ecosystems: abundance, characterization, and sources in two major reservoirs

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Microplastic (MP) contamination is a global concern, yet its impact on Sri Lanka's reservoirs remains largely unexplored. These reservoirs provide vital ecosystem services and regulate river runoff. This study examines MP concentrations, characterization, and their spatial distribution in Samanalawewa and Udawalawe reservoirs in the Walawe River Basin, where human activities significantly contribute to MP pollution. Random sampling was employed at 11 locations in Samanalawewa during February 2024 and at 15 locations in Udawalawe in October 2024. MP analysis was conducted through imaging with Nile-Red stain method. MPs were detected in both surface and bottom (10 m depth) water collected from the studied reservoirs, with a total of 156 samples across different sites. The study found that blue MPs were the most frequently presented in both reservoirs, accounting for 35.2% of particles in Samanalawewa and 38.6% in Udawalawe. In terms of morphology, fibers were more prevalent in the Udawalawe Reservoir, accounting for 73.4%, compared to 34.7% in the Samanalawewa reservoir. The size of the MPs ranged between 0.05 mm and 5 mm. Fishing activity are much higher in Udawalawe reservoir than Samanalawewa reservoir. The observed abundance

of MPs in Udawalawe reservoir ((surface:  $3.44 \pm 1.06$  particles / L), and (bottom:  $1.87 \pm 1.04$  particles / L)) is higher than that in Samanalawa reservoir ((surface:  $2.36 \pm 1.9$  particles / L), (bottom:  $0.77 \pm 0.97$  particles / L)). This may also have been the reason for the increase in the percentage of fibers in the Udawalawe reservoir. The source of MPs' depends on local human activities (fishing, tourism and agriculture). This study reveals MP contamination in inland Sri Lanka, highlighting its widespread impact. Findings establish a baseline for MP pollution in the Walawe river basin and stress the urgent need for better waste management and sustainable water use to protect these ecosystems.

# Keywords:

Microplastics; freshwater ecosystem; reservoirs; morphology; Walawe river basin

# Acknowledgment:

Grants received from The Centre for Environment, Fisheries and Aquaculture Science (Cefas) under the Ocean Country Partnership Program (OCCP) of the Blue Planet Fund is acknowledged.

# Development of 8-hydroxyquinoline derivatives as fluorescence sensors for Zn<sup>2+</sup> detection

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Zinc (Zn<sup>2+</sup>) is the second most abundant transition metal ion in the human body and plays a crucial role in numerous biological, environmental, and industrial processes. This study aimed to synthesize ester derivatives of 8-hydroxyquinoline (8-HQ), develop them as fluorescent chemosensors, and investigate their selectivity towards Zn<sup>2+</sup> ions. Three 8-HQ ester derivatives; (8-hydroxyquinolin-5-yl)methyl benzoate (1), (8-hydroxyquinolin-5-yl)methyl 4-methoxybenzoate (2), and (8-hydroxyquinolin-5-yl)methyl 4-trifluoromethylbenzoate (3) were successfully synthesized as fluorescent sensors for Zn<sup>2+</sup> detection. The synthesis involved a two-step process: first, 8-HQ was converted to 5-hydroxymethyl-8-hydroxyquinoline (5-HMHQ); subsequently, Steglich esterification was performed using benzoic acid and para-substituted benzoic acids (-OCH<sub>3</sub> and -CF<sub>3</sub>) as carboxylic acid components and 5-HMHQ as the alcohol component. The coupling reagent N,N'-dicyclohexylcarbodiimide (DCC) and the catalyst 4-dimethylaminopyridine (DMAP) were used in CH<sub>2</sub>Cl<sub>2</sub> at room temperature. The by-product, dicyclohexylurea (DCU), was removed via acid washing followed by column chromatography. The absorption spectra of the derivatives displayed two distinct peaks corresponding to the free and Zn<sup>2+</sup>-complexed forms at the wavelengths 317 nm and 400 nm for (1), 316 nm and 393 nm for (2), 318 nm and 397 nm for (3). Fluorescence emission spectra, obtained upon excitation at the absorption maxima of the free probes; 317 nm for (1), 316 nm for (2), and 318 nm for (3), revealed fluorescence quenching and the formation of metal-ligand complexes upon Zn<sup>2+</sup> addition. All three compounds exhibited iso-emissive points in their emission spectra, indicating equilibrium between free and bound forms, with metal-to-ligand binding stoichiometries of 1:1, 1:2, and 1:3. These results demonstrate that the synthesized 8-HQ derivatives are effective fluorescent probes for the sensitive and selective detection of Zn<sup>2+</sup> ions through ratiometric response and fluorescence enhancement.

### Keywords:

8-hydroxyquinoline ester derivatives; Zn<sup>2+</sup>; Steglich esterification; fluorescent chemosensors

# Development of dual-carrier CMC-PEG/LDH nanocomposite hydrogel for the sustained release of *Mikania cordata* phytochemicals

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Mikania cordata (Burm. f.) B.L. Robinson is a medicinal plant of the Asteraceae family, demonstrating antiinflammatory, antimicrobial, and wound-healing properties. However, poor bioavailability due to instability and rapid clearance of its phytochemicals hinders its potential. This study developed a dualcarrier nanocomposite hydrogel system composed of Mg-Al layered double hydroxide (LDH) nanoparticles and citric acid crosslinked carboxymethyl cellulose (CMC)-polyethylene glycol (PEG) hydrogel for the sustained release of M. cordata phytochemicals. Pristine LDH was synthesized by the co-precipitation method by mixing Mg(NO<sub>2</sub>)<sub>2</sub>.6H<sub>2</sub>O and Al(NO<sub>2</sub>)<sub>2</sub>.9H<sub>2</sub>O at a 2:1 molar ratio under a nitrogen atmosphere at pH 10. The leaves were extracted via ethanol maceration, and the plant extract was loaded into LDH using the solventassisted ion exchange method. The resulting MC-LDH nanocomposite was incorporated into the hydrogel by incorporating a MC-LDH suspension in a CMC and PEG (2:1.2 w/w) blend through in situ gelation and crosslinking with citric acid (20% w/CMC). Structural characterizations using FTIR, UV-Vis, and XRD suggest the presence of phytochemicals in the

plant extract and their potential intercalation into the LDH structure while preserving LDH crystallinity. An increase of +0.599 Å in basal spacing (d<sub>003</sub>) and a nearconstant d<sub>110</sub> support the likelihood of guest molecule intercalation while maintaining LDH structural integrity. The presence of FTIR peaks in MC-LDH that resemble those of the M. cordata extract, and are absent in pristine LDH, supports the possible intercalation of phytochemicals with the LDH matrix. Encapsulation efficiencies were 81.53% for LDH and 72.89% for the hydrogel (p < 0.05), demonstrating strong loading capacity. Swelling studies showed excellent water absorption (162%). Drug-release profiling revealed that the hydrogel significantly prolonged release compared to MC-LDH alone, releasing only 70% in 3 hours versus 95% from MC-LDH (p < 0.001), confirming dual-stage sustained release behavior. The system demonstrates strong potential as a wound dressing material.

### Keywords:

*Mikania cordata*; LDH nanocomposite; hydrogel; sustained release; wound dressing

# Abundance and characterization of microplastics in *Dawkinsia filamentosa* inhabiting the Kothmale reservoir, Mahaweli upper catchment in Sri Lanka

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Microplastics (MP) are plastic particles less than 5 mm in size, and it is an emerging pollutant with a rising global concern. Reservoirs are considered an enclosed aquatic environment, and the presence of MP in the freshwater environment poses a serious risk to its biota. Recent studies have used fish species as bio-indicators to monitor microplastic contamination in reservoirs. Most such studies have been conducted based on marine habitats, while limited research has been done in freshwater environments. In this study, 78 samples from the Dawkinsia filamentosa (in Sinhala "Pulli tittaya") fish species caught by the local fishermen from Kothmale reservoir in Sri Lanka, in July and October 2024 were analyzed. MPs extracted from gastrointestinal tracts (GI) and the gills (GL), were digested in KOH and vacuum filtered. Stereomicroscope equipped with a micro-imaging software was employed for the analysis of the isolated MPs. A total of 51 MP particles were detected in the fish samples analyzed, out of which, 28 (54.90%) were in the gills and 23 (45.10%) were in the digestive tracts of the fish samples. The average MP abundance in the gills was  $0.72 \pm 0.85$  items per gram, while that in the digestive tracts was  $0.30 \pm 0.54$  items

per gram. The most abundant shapes of MP particles were fibers found in the gills (89%) and in the digestive tracts (74%) followed by fragments. Among them, the prevailing colours of MPs were blue, black, red and green. Herein, the gills had the highest concentration of MPs in blue (50%), whereas most of the MPs found in the digestive tracts also were in blue (48%). The most frequent size (0.1 - 1 mm) in the gills and digestive tracts were 57% and 48 %, respectively. These findings revealed that a significant microplastic contamination in *Dawkinsia filamentous* can pose potential risks to its consumers and impact the other aquatic environments.

### Keywords:

Microplastics; *Dawkinsia filamentosa*; Kothmale reservoir; digestive tract; gills

# Acknowledgement:

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# Nano-crystalline hydroxyapatite from scales of the reef fish Epinephelus malabaricus (galkossa)

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Fish scales comprise of collagen and hydroxyapatite (HAp). The latter of which holds potential for biomedical applications. In Sri Lanka these scales are discarded into the environment as waste. The objective of this research was to develop a method to prepare nanocrystalline HAp from scales of the reef fish Epinephelus malabaricus (Gal Kossa). Scales were collected from Ja-Ela, Sri Lanka, washed, dried and subjected to acid deproteinization with hydrochloric acid (HCl) under varying conditions (concentrations: 0.1 M, 0.2 M; temperatures: room temperature, 60 °C; treatment periods:1 h, 2 h). The product was isolated, washed and dried. The best conditions were treatment with 0.2 M HCl at 60 °C for 2 h. The product was subjected to alkaline deproteinization under different conditions (NaOH gave better results than KOH; NaOH concentrations: 2%, 3%, 4%, 5% w/v; temperature: 60 °C, 70 °C; treatment periods: 1, 2 and 3h.). The product was isolated, washed and dried. The best condition was treatment with 4% NaOH at 70 °C for 3 h. The product was subjected to alkaline heat treatment using NaOH under different conditions. (concentration: 20%, 25%,

30% w/v; temperature: 60 °C, 80 °C; treatment period: 1h, 2 h, 3 h). The product was isolated, washed and dried. The best condition was 25% NaOH at 80 °C for 2 h. Under the best conditions for acid deproteinization, alkaline deproteinization and alkaline heat treatment, the yield was 43%. Characterization using FT-IR and XRD analysis of the product confirmed the product as hydroxyapatite. According to EDX, Ca/P ratio was 1.82. SEM showed agglomerated particles within 100 nm range. The FT-IR suggested it to be a B-type carbonated hydroxyapatite (CO<sub>2</sub><sup>2-</sup> groups at 1462, 1417 and 873 cm<sup>-1</sup>) where CO<sub>3</sub><sup>2-</sup> ions substituted in place of certain  $PO_4^{3-}$  ions. TGA confirmed the carbonated form. Therefore, this method can be used as a cost-effective method to produce pure carbonated hydroxyapatite. It also helps to reduce the environmental pollution due to fish waste.

### Keywords:

Fish scales; nano-crystalline; hydroxyapatite; deproteinization; biocompatibility

# Electroanalytical detection of imidacloprid on stearic acid modified glassy carbon electrode

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Extensive use of pesticides in modern agriculture has become a hidden global threat. Imidacloprid, which is one of the world's most widely used insecticides poses a serious impact on the environment due to its long term persistence in groundwater and soil. In addition, contamination of food with imidacloprid residues can pose health risks to both humans and animals. Hence, its detection in environmental and food samples is essential. Among various analytical techniques, electroanalytical techniques offer a simple and cost effective method for imidacloprid detection. In this study, a simple, cost effective electrochemical method based on stearic acid was developed for the determination of imidacloprid. Stearic acid is non electro-active hence, it forms a barrier on the electrode surface preventing electrode fouling, improving the analytical performance of the electrode. It acts as a cost effective electrode modifier when compared to some commonly used electrode modifiers such as metal nanoparticles, metal oxides, and carbon nanotubes. The glassy carbon electrode was modified with stearic acid using simple drop casting method. Electroanalytical

techniques such as cyclic voltammetry and steady state amperometry were utilized to investigate the electrochemical behavior of imidacloprid at the stearic acid modified glassy carbon electrode. Cyclic voltammetric analysis results in a single reduction peak at -1.2 V, indicating the electro-activity of imidacloprid. In amperometric studies, the noise level observed with the bare electrode has significantly reduced with the modification of the electrode with stearic acid. Therefore, the developed modified electrode provides an amperometric sensor for detection of imidacloprid with a linear dynamic range of 1.19 x 10<sup>-4</sup> mol dm<sup>-3</sup> to 6.97 x 10<sup>-4</sup> mol dm<sup>-3</sup>. The proposed amperometric sensor exhibited a minimum detection limit of 6.81 x 10<sup>-5</sup> mol dm<sup>-3</sup> and a limit of quantification of 2.27 x 10<sup>-4</sup> mol dm<sup>-3</sup>, offering a potential tool for imidacloprid detection in environmental samples.

## Keywords:

Amperometry; cyclic voltammetry; modified electrode; stearic acid

# Determination of rainwater quality at selected locations in Kandy district

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Chemical characteristics of atmospheric deposition, the major pathway for washing out pollutants from the atmosphere to the earth's surface, can be determined using bulk deposition, whose composition would be used to identify the atmospheric quality of selected locations. Although the determination of the quality of surface water is a common exercise, analysis of rainwater has not been given due attention despite the necessity of having a nationwide rainwater quality database. In this respect, this study was focused on the determination of rainwater quality through the analysis of bulk deposition weekly collected from April to November 2024, at three sampling sites: the University of Peradeniya (UOP), the Kandy Zonal Educational Department (KED), and the Polgolla Mahaweli Authority (PMA) Premises. The water quality parameters, namely, rainfall, pH, conductivity, total dissolved solids (TDS), total hardness, anionic species: Cl<sup>-</sup>, NO<sub>3</sub><sup>-</sup>, SO<sub>4</sub><sup>2-</sup>, and trace elements: Fe, Zn, Cu, Cr and Pb, determined with the aid of standard analytical procedures throughout the period indicate

that the Kandy sampling site, having the lowest average pH (min: 5.21; max 8.34) and the highest average values for many quality parameters, was the most polluted region, due to the urbanization and low vegetation cover. Moreover, a smaller number of dry deposition events occurred at each sampling site, with an overall value of 12.6 %. Anions of bulk deposition followed the trend,  $Cl^{-} > SO_{4}^{2-} > NO_{3}^{-}$  at the UOP and PMA sampling sites, while the KED site followed Cl<sup>-</sup> > NO<sub>3</sub><sup>-</sup> > SO<sub>4</sub><sup>2-</sup>. Nevertheless, the trace metal concentration of all sampling sites showed the trend, Fe > Cu > Zn > Cr > Pb. The Pearson correlation coefficient of conductivity, TDS, and total hardness shows a positive correlation each other, while rainfall and pH inversely correlate with each other. Sulphate and chloride anions at three sampling sites are positively correlated, and Zn, Cu, and Cr show a positive correlation with each other.

# Keywords:

Bulk deposition; Kandy; pearson correlation; rainwater; urbanization

# Synthesis and determination of *in-vitro* anti-urolithiatic activity of quinazolinone derivatives

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Quinazolinone derivatives are a group of heterocyclic compounds known for their diverse biological activities and pharmaceutical applications. However, the potential of quinazolinone-based compounds preventing or treating urolithiasis remains in unexplored. Therefore, this study primarily focused on the synthesis and investigation of the in-vitro antiurolithiatic activities of quinazolinone derivatives, including 2-(2-methoxyphenyl)-3H-quinazolin-2-(2-hydroxyphenyl)-3H-quinazolin-4-4-one, one, 2-(3-hydroxyphenyl)-3H-quinazolin-4-one, 2-(4-hydroxy-3-methoxyphenyl)-3H-quinazolin-4and 2-(4-nitrophenyl)-3*H*-quinazolin-4-one. one, Quinazolinone derivatives were synthesized via oxidative cyclo-condensation of 2-aminobenzamide with substituted aldehydes utilizing FeCl<sub>3</sub> as a Lewis acid catalyst. The structures of the synthesized analogues were confirmed using spectroscopic techniques including Fourier-transform infrared spectroscopy, <sup>1</sup>H-NMR, <sup>13</sup>C-NMR, and high-resolution mass spectrometry. In-vitro anti-urolithiatic activity of the synthesized derivatives was evaluated in triplicates using calcium oxalate crystal initiation assay, calcium oxalate crystal growth assay, and calcium oxalate crystal aggregation assay. Statistical analysis was performed using the one-way ANOVA test. Among the tested compounds, 2-(2-methoxyphenyl)-3H-quinazolin-4-one demonstrated the highest crystal initiation inhibition activity, with lowest IC<sub>50</sub> value (352.23  $\pm$  16.29  $\mu$ g/mL) outperforming the standard potassium citrate (593.52  $\pm$  53.78 µg/mL); followed by 2-(3-hydroxyphenyl)-3H-

quinazolin-4-one (392.67  $\pm$  9.86 µg/mL), 2-(4-hydroxy-3-methoxyphenyl)-3*H*-quinazolin-4-one (461.84  $\pm$ 26.17 µg/mL), 2-(4-nitrophenyl)-3H-quinazolin-4-one (521.89 ± 119.46 µg/mL), and 2-(2-hydroxyphenyl)-3H-quinazolin-4-one (528.31 ± 16.29 µg/mL). The highest crystal growth inhibition activity was exhibited by 2-(2-methoxyphenyl)-3H-quinazolin-4-one  $(330.47 \pm 9.76 \,\mu\text{g/mL})$  compared to potassium citrate  $(771.09 \pm 22.67 \ \mu g/mL)$ ; followed by 2-(4-hydroxy-3-methoxyphenyl)-3*H*-quinazolin-4-one (466.44  $\pm$ 40.77 µg/mL), 2-(3-hydroxyphenyl)-3H-quinazolin-4-one (660.33 ± 17.83 µg/mL), 2-(4-nitrophenyl)-3H-quinazolin-4-one (691.49  $\pm$  3.54 µg/mL), and 2-(2-hydroxyphenyl)-3H-quinazolin-4-one (691.49  $\pm$  32.23 µg/mL). In the crystal aggregation assay, the IC<sub>50</sub> values of 2-(3-hydroxyphenyl)-3H-quinazolin-4one, 2-(4-hydroxy-3-methoxyphenyl)-3H-quinazolin-2-(2-hydroxyphenyl)-3H-quinazolin-4-one, 4-one, 2-(2-methoxyphenyl)-3H-quinazolin-4-one, and 2-(4-nitrophenyl)-3H-quinazolin-4-one were reported as  $455.84 \pm 5.48 \ \mu g/mL$ ,  $501.64 \pm 13.33 \ \mu g/mL$ , 521.41 $\pm$  44.37 µg/mL, 545.57  $\pm$  8.78 µg/mL, and 634.50  $\pm$ 47.41 µg/mL, respectively. Potassium citrate, used as the standard, showed an IC<sub>50</sub> value of 333.33  $\pm$  12.39 µg/mL. These findings highlight the potential of quinazolinone derivatives as promising candidates for urolithiasis treatment.

### Keywords:

Anti-urolithiatic activity; quinazolinone derivatives; initiation assay; growth assay; aggregation assay

# A novel energy-efficient method to produce crystalline silica from burnt rice husk ash

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The sol-gel method is efficient and sustainable for synthesizing high-purity silica from rice husks (RH), commonly available agricultural waste. Silica is a widely used material in various commercial applications for absorbing and retaining moisture. Producing commercial silica is costly and energy-intensive. In this study, we produced silica from rice husk ash (RHA) using the alkaline treatment. In the conventional alkaline treatment, silica is extracted as a water-soluble sodium silicate (Na<sub>2</sub>SiO<sub>3</sub>) solution by heating RHA with sodium hydroxide (NaOH). Then this solution is filtered and acid-treated until neutralization, until the silica aerogel is formed. In this work, we produced Na<sub>2</sub>SiO<sub>3</sub> solution with 3M NaOH under 360 W microwave at 100 °C for 25 minutes. Silica aerogel is produced using the indirect neutralization method. Here, an excess of 1M Hydrochloric acid (HCl) was added to the Na<sub>2</sub>SiO<sub>3</sub> solution to lower the pH to 2.5. Then, 1M NaOH was used to increase the pH back to 7, where the aerogel is formed. Silica yield was 74.4% from acid-treated

black rice husk ash. The FT-IR spectrum of RHA silica shows four major peaks. According to SEM-EDX and XRF, our RHA silica contains 82.21% silica. In contrast, all other elements, Al, Ca, Fe, Mn, and K, account for only 1.19% of the sample. The remaining 16.6% consists of sodium (Na) and chlorine (Cl), with no carbon residues detected in the sample according to TGA. The XRD analysis reveals sharp peaks at 2Theta values of 27.40°, 28.64°, 40.84°, 45.53°, 53.90°, 56.50°, 66.22°, and 75.34° indicating strong crystalinity with 78.38%. The particle size analysis revealed an average particle size is 15.99 µm. Microwave heating is used for alkaline treatment because it is more energy efficient compared to other heating methods. This proposed novel method produced crystalline silica from burnt rice husk ash without requiring high-temperature heating.

## Keywords:

Burnt rice husk ash; sol-gel method; indirect neutralization; silica; crystalline

# Novel Zr(IV) and Hf(IV) – Schiff base complexes as white light photocatalysts for the degradation of methylene blue

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Untreated dyes found in industrial effluent damage aquatic habitats and diminish biodiversity. Therefore, dye-containing hazardous substances must be treated before being disposed of. Nowadays, TiO<sub>2</sub>, ZnO, metal niobates and titanates, as well as other semiconductors with a large band gap, serve as the foundation for extensively used UV photocatalytic materials with high performance. To produce novel photocatalysts with excellent efficiency under white light, zirconium(IV) and hafnium(IV) Schiffbase complexes were synthesized and studied to determine their potential as photocatalysts for the degradation of methylene blue (MB) dye. The Schiff base, H<sub>2</sub>(Sal)<sub>2</sub>(hexamethylenediamine) (SB) ligand, a yellow crystalline solid (m. p. 65 °C, 18.45%) was synthesized by the condensation of salicylaldehyde and hexamethylenediamine. Coordination complexes of Zr(IV) and Hf(IV) were synthesized by mixing M:SB in 1:2 ratio to obtain light yellow and orange solids with yields of 58.8% and 6.5%, respectively, and both exhibit high thermal stability with melting points above 300 °C. The characterization of both complexes was conducted through Fourier-transform infrared spectroscopy (FTIR). The three-dimensional structures of the complexes were predicted using sophisticated computer modeling. Additionally, the ORCA 5.0 code, the hybrid B3LYP functional, and the def2-TZVP basis set were used for calculations in the aqueous phase. The catalytic efficacy of the Zr(IV) and Hf(IV) Schiff base complexes

for the degradation of methylene blue (MB) was systematically examined under white light irradiation for varying durations (30, 60, 90, 120, and 150 minutes) using UV-Vis spectroscopy. The study was conducted both in the absence and presence of different volumes of 30% H<sub>2</sub>O<sub>2</sub> (0.1, 0.15, and 0.2 mL) to investigate the role of H<sub>2</sub>O<sub>2</sub> in enhancing the catalytic performance. The complexes' strong metal-ligand interactions, excellent thermal stability, and favorable electronic characteristics contribute to their increased activity. Overall, this study demonstrates that the synthesized metal complexes act as excellent photocatalysts in the presence of H<sub>2</sub>O<sub>2</sub> for organic dye degradation, offering an environmentally benign method of wastewater treatment. In conclusion, Zr(IV) and Hf(IV) Schiff base complexes showed the highest degradation percentage of methylene blue after 150 minutes with 0.2 mL of 30% hydrogen peroxide, 73% and 82%, respectively. Further research into understanding mechanistic pathways may improve their practical applicability in industrial wastewater treatment.

### Keywords:

Zirconium; Hafnium; Schiff base ligand; photocatalysis

#### Acknowledgments:

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# Comprehensive physicochemical characterization and bioactivity assessment of Rajata Bhasma as a multi-target therapeutic agent

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Rajata Bhasma (RB) is a traditional Ayurvedic herbometallic preparation used to treat neurological disorders, aging, cardiac and circulatory disorders, fever and infections. Due to the paucity of standardized data in the literature, physicochemical characterization was undertaken to ensure the quality and consistency of Rajata Bhasma. RB contains 0.12±0.01% moisture, 83.2±0.2% total ash, 75.1±0.3% acid-insoluble ash, and 25.4±0.1% water-soluble ash. X-ray diffraction confirmed the predominant crystal structure as Ag<sub>2</sub>S, with an average particle size of 21.4±0.4 µm. Scanning electron microscopy showed irregular granular surface morphology, suggesting a mixture of compounds beyond Ag<sub>2</sub>S. Energy-dispersive X-ray spectroscopy detected additional elements including O(21.26%), C(5.76%), Na(3.98%), Si(0.33%), and Fe(1.83%). Thermogravimetric analysis indicated the presence of composite materials with varying thermal degradation temperatures, while FT-IR confirmed Ag-S bonds, C-O bonds, and hydroxyl groups, likely attributable to the plant compounds used during preparation. RB exhibited 40% DPPH radical scavenging activity at 200 µg/mL) compared to standard BHT. It demonstrated an antidiabetic potential with alpha-glucosidase inhibition  $(IC_{50}=2.10\pm0.03 \ \mu g/mL)$ , surpassing the standard acarbose (IC<sub>50</sub>=200.9±0.4 µg/mL), and significant (P<0.05) alpha-amylase inhibition (IC<sub>50</sub>=42.8 $\pm$ 0.2 µg/mL). RB showed notable lipase inhibition

(IC<sub>50</sub>=110.2 $\pm$ 0.7 µg/mL) compared to standard orlistat and anti-inflammatory potential (IC<sub>50</sub>=220.9±1.8 µg/ ml) compared to aspirin. Antibacterial assessment revealed an activity against B. subtilis with inhibition zones of 19.01±1.41 mm at 2.5 mg and 25.06±1.41 mm at 5 mg, compared to amoxicillin (14.01±1.41 mm at 0.1 mg). Against E. coli, RB showed moderate activity with inhibition zones of 16.30±1.53 mm at 2.5 mg and 23.30±0.58 mm at 5 mg, compared to amoxicillin (31.30±0.58 mm) at 0.05 mg. For S. aureus, RB exhibited inhibition zones of 15.70±0.58 mm at 2.5 mg and 22.00±1.00 mm at 5 mg, while amoxicillin showed 35.70±0.58 mm at 0.05 mg. RB possesses diverse bioactivities and a complex physicochemical profile which supports its potential applications in the treatment of metabolic syndrome, diabetes, inflammation, and bacterial infections. Further studies to assess the above activities in vivo will reveal the true potential of RB on these disorders mentioned.

#### Keywords:

Rajata Bhasma; anti-diabetic activity; anti-bacterial activity; physicochemical characterization; enzymatic inhibition

### Acknowledgement:

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# Standardization and bioactivity evaluation of a distillate from a traditional herbal formula

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This study aimed to standardize and evaluate the bioactivity of a distillate prepared from a traditional herbal formula using Phyllanthus emblica Linn, Tinospora cordifolia, and Aerva lanata var. rotundifolia. Standardization parameters assessed included colour, odour, pH, total solid content, ethanol content, viscosity, and specific gravity. The distillate was colourless with an aromatic odour, had a pH of  $4.64 \pm 0.06$ , and showed no detectable solid content, indicating its predominantly volatile composition. The alcohol content of the distillate at 25 °C (v/v%) was 0.49±0.14%; determined by specific gravity. Also, no detectable viscosity was observed. Microbial contamination tests revealed aerobic plate count (APC) values of 5666.7 CFU and yeast and mold count (YMC) of 3.6 CFU, both within acceptable limits, ensuring microbiological safety. Pathogenic bacteria, including Escherichia coli, Salmonella spp., Staphylococcus aureus, and Pseudomonas aeruginosa, were not detected. No heavy metals or sugars were detected. The phytochemical analysis of ethyl acetate extract of the distillate (EAED), obtained through solvent partitioning, revealed a total phenolic content of  $1.55 \pm$ 0.06 mg/g GAE, total flavonoid content of  $2.36 \pm 0.09$ mg/g, and total condensed tannin content of 0.76  $\pm$ 0.24 mg/g. EAED demonstrated significant antioxidant

activity, with DPPH assay showing higher radical scavenging activity (182.47  $\pm$  6.23 µg/mL) compared to the BHT standard ( $52.04 \pm 4.68 \,\mu g/mL, p < 0.05$ ). The FRAP assay confirmed antioxidant potential with mean absorbance of 0.251  $\pm$  0.002 compared to BHT: 0.514  $\pm$ 0.009. Human Red Blood Cells membrane stabilization assay showed anti-inflammatory activity: EAED (IC50:  $807.16 \pm 22.39 \ \mu g/mL$ ), aspirin (IC<sub>50</sub>:  $88.85 \pm 2.14 \ \mu g/mL$ ) mL). Acute toxicity testing using Moina macrocopa indicated a safe LC50 value of 22.26 ppm, suggesting a favourable safety profile. HPLC analysis of the ethyl acetate extract identified 9 major compounds. In conclusion, the distillate from this traditional herbal formulation exhibits strong antioxidant activity, microbiological safety, and potential as a bioactive product.

### Keywords:

Traditional herbal formula; antioxidant activity; phytochemical analysis; microbial contamination; acute toxicity

## Acknowledgment:

This research is funded by Hettigoda Industries and National Research Council of Sri Lanka.

## Standardization, phytochemical profiling, and bioactivity evaluation of a traditional herbal tea bag formulation

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This study investigates the standardization and bioactivity of a tea bag formulated from a Traditional Herbal Formula (THF) composed of Nelli (Phyllanthus emblica), Rasakinda (Tinospora cordifolia), and Polpala (Aerva lanata var. rotundifolia). The formulation met quality standards with a moisture content of 9.0% and total ash of 5.77%. Phytochemical extraction showed higher recovery yields in methanol extract (ME) as 12.7% compared to water extract (WE) as 9.35%. ME exhibited significantly higher Total Phenolic Content (TPC) as 25.61±0.97 mg GAE/g and Total Flavonoid Content (TFC) as 6.31±0.6 mg/g than WE having TPC and TFC values as 8.13±0.13 mg GAE/g and 2.93±0.108 mg/g, respectively. Total Condensed Tannin Content was comparable between ME and WE as 3.60±0.293 mg/g and 3.55±0.324 mg/g, respectively. Antioxidant assays confirmed strong free radical scavenging potential. ME exhibited an IC<sub>50</sub> of 1118.96±23.33 µg/ mL (ABTS) and 6.67±0.049 µg/mL (DPPH), whereas WE showed 1729.25±43.85 µg/mL (ABTS) and 9.22±0.40 µg/mL (DPPH) comparable to standard BHT 505.66±3.12 µg/mL (ABTS), 52.04±4.68 µg/mL (DPPH). The mean absorbance values of FRAP assay obtained from BHT, ME and WE were 0.577±0.065, 0.595±0.007, and 0.465±0.009, respectively. Antiinflammatory activity was observed with IC<sub>50</sub> values

of 70.56±1.56 µg/mL (ME) and 270.16±6.92 µg/ mL (WE), comparable to aspirin 66.90±6.54 µg/mL. Acetylcholinesterase inhibition was significant, where IC<sub>50</sub> of ME was 438.92±7.84 µg/mL and 915.01±1.68 µg/mL in WE, compared to 137.43±0.89 µg/mL for donepezil. Alpha-glucosidase inhibition assay showed IC50 of 206.73±19.01 µg/mL in acarbose, 158.77±27.66 µg/mL in ME, 124.49±10.60 µg/mL in WE. Alphaamylase inhibition at 500 µg/mL showed 21.61% in ME, 12.5% in WE compared to 96% for acarbose. Xanthine oxidase inhibition was highest in ME (43.98% at 500 µg/mL). Microbiological analysis showed aerobic plate count and yeast/mold counts were within permissible limits. These findings suggest the THF-based tea bag is a potent herbal product with significant antioxidant, anti-inflammatory, and enzyme-inhibitory properties.

#### Keywords:

Traditional herbal formula; phytochemical analysis; antioxidant activity; medicinal plants; bioassays

### Acknowledgment:

This research is funded by Hettigoda Industries and the National Research Council of Sri Lanka.

## Evaluation of the *in vitro* bioactive potential of *Salicornia brachiata* for therapeutic applications in metabolic disorders

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Salicornia brachiata belongs to the genus Salicornia, which has halophytic characteristics and exhibits important therapeutic potential besides its phytochemical richness. This research aims to evaluate the biological activities of methanolic extract (ME), chloroform extract (CE), and hexane extract (HE) obtained from S. brachiata aerial plant parts to evaluate their potential as natural therapeutic agents. Fresh plant materials were collected from salt marshes in the Mannar district, Sri Lanka. Multiple in vitro tests showed antihypertensive together with antidiabetic, anti-obesity, antioxidant, and neuroprotective effects angiotensin-converting through enzyme (ACE) inhibition, a-glucosidase inhibition, pancreatic lipase inhibition, xanthine oxidase inhibition and acetylcholinesterase enzyme inhibition assessments. The inhibitor concentrations of 0.5 mg/mL showed ACE inhibition amounts at 59.24±0.78% (ME) and 72.87±1.67% (CE) while HE displayed a lower value of 51.56±1.37% when compared to captopril with 90.56 $\pm$ 2.77% inhibition. Meanwhile, for  $\alpha$ -glucosidase inhibition tests, ME and HE had inhibition rates of 09.23±0.76% and 48.97±3.28% respectively whereas CE exhibited 73.89±2.69% inhibition alongside acarbose at 71.12±2.69% inhibition. The extracts inhibited pancreatic lipase to various extents:

58.67±1.59% inhibition for ME, 18.78±4.85% for CE and 21.09±0.85% for HE whereas orlistat showed 88.78±0.97% inhibition. The xanthine oxidase inhibition assay measured antioxidant activity through inhibitor activity percentages of 22.14±2.67% (ME), 39.69±1.73% (CE), and 21.38±0.97% (HE) while the standard inhibitor allopurinol yielded an inhibitor activity of 79.0±0.88%. The inhibitory effects on acetylcholinesterase measured 22.98±1.23% (ME), 35.55±5.1% (CE) and 38.21±1.23% (HE). while donepezil displayed 55.91±0.78% inhibition. These results confirm that S. brachiata possesses useful bioactive compounds which show potential for use as antihypertensive and antidiabetic pharmaceutical agents. The research findings support the growing interest in using natural products for disease conditions associated to modern lifestyles.

#### Keywords:

Antihypertension, antidiabetic, *in vitro* bioactivity, halophyte, metabolic disorders

### Acknowledgements:

This research was funded by the Asian Development Bank (Grant No: CRG/R2/RJ1).

## Analysis of malachite green adsorption on multiple coated graphite oxide/ sand (M-GO/S) composite by incorporating isotherm and kinetic studies

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The increasing discharge of toxic dyes from industrial effluents into aquatic environments poses a severe threat to ecosystems and public health due to the nonbiodegradable and carcinogenic nature. This research focuses to investigate the potential suitability of multicoated graphene oxide-sand (M-GO/S) composite material for removal of malachite green (MG). This composite material was synthesized by 5-time coating of graphene oxide layers on purified river sand using a thermal annealing process. Synthesized composite was characterized by Scanning Electron Microscopy (SEM) and Fourier-Transform Infrared Spectroscopy (FT-IR). In this study, the effects of experimental parameters such as initial MG concentration, pH, composite dosage, and shaking time on MG adsorption were evaluated at room temperature via batch adsorption experiments. Then utilizing these optimized conditions, isotherm and kinetic studies were conducted on MG adsorption by the adsorbent and experimental analysis were triplicated. Post-shaking, dye concentration in the supernatant was measured using a UV-Vis spectrophotometer at 617 nm, enabling the determination of MG removal

percentages. According to the SEM results, composite appeared as irregularly shaped granules with nonuniform GO coating on the sand surface, while FT-IR outcomes revealed presence of oxygenated functional groups on the surface. Adsorption results indicated the highest MG removal percentage with initial MG concentration (3 mg/L), pH (5), M-GO/S dose (0.09 g), and shaking time (40 min). Among the two isotherm models, the Langmuir isotherm (R<sup>2</sup> =0.9404) is better fitted with data having a maximum adsorption capacity (Q<sub>max</sub>) of 0.4840 mg/g. Furthermore, kinetic studies revealed the better match with pseudo second order kinetics (R<sup>2</sup>=0.9218). These findings revealed that the adsorption mechanism primarily comprises monolayer adsorption by means of a chemical sorption process. Ultimately, these findings suggest that the novel composite could be a promising solution for the removal of positively charged dye molecules such as MG from contaminated water.

### Keywords:

Adsorption; graphene oxide; isotherm; kinetics

## Investigation of curry leaves (*Murraya koenigii*) as a sustainable biosorbent for cadmium removal in aqueous solutions

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The presence of cadmium in food sources creates significant health hazards due to its toxic nature and inability to decompose naturally. Despite the development of various solutions for contaminant removal from food items, there is a significant demand for cost-effective and efficient biosorbents, particularly in the context of food preparation. This research conducts a preliminary study on how curry leaves can serve as an effective biosorbent for cadmium removal from aqueous solutions, which is beneficial for exploring their potential as a biosorbent in food preparation. Curry leaves were collected from Kurunegala district, Sri Lanka and subsequently, washed, dried and ground to <1 mm particle size. Batch adsorption studies were conducted by varying the parameters such as initial cadmium concentration, pH, adsorbent dosage, and shaking time. Isotherm and kinetic studies were then performed using the obtained optimized conditions. All analyses were performed using Inductively Coupled Plasma-Mass Spectroscopy and conducted triplicates. This study showed an improvement in removal efficiency when increasing initial cadmium concentration and obtained peak removal at 0.6

ppm concentration. pH and adsorbent dosage were optimized at 3.0, and 0.05 g having removal efficiencies of 70.2% and 61.5%, respectively. The best contact time found was 120 minutes (70.83%). The experimental data showed the best match with the Langmuir model during adsorption isotherm analysis ( $R^2 = 0.9373$ ) which indicated monolayer adsorption on a homogeneous surface. The adsorption kinetic was pseudo-secondorder (R<sup>2</sup>= 0.9814) which indicates chemisorption as the rate-determining step. The maximum adsorption capacity of curry leaves was 6.93 mg/g. Furthermore, according to the equilibrium parameter (RL <1) in this study, indicates a favorable Cd adsorption by curry leaves. The study reveals that curry leaves have a better cadmium removal capacity, offering a natural solution for reducing cadmium toxicity in aqueous solution, indicating further need for investigation under food preparation conditions.

## Keywords:

Curry leaves; Cadmium; bio-adsorption; isotherm; kinetic modeling

## Evaluation of *Garcinia quaesita* fruit rinds as a sustainable biosorbent for effective cadmium removal

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The presence of toxic heavy metals such as cadmium in water sources, particularly those used for consumption, cause a significant threat to human health. The use of contaminated water in food preparation can lead to the accumulation of toxic metals in food items and then finally in human body. Therefore, exploring biosorbents that are effective and suitable for culinary applications has become an important need. The present study examines the adsorption capability of Garcinia quaesita (commonly known as Goraka) and its potential as a sustainable biosorbent. G. quaesita fruit rinds collected from Panadura district, Sri Lanka, were washed, dried, and pulverized to <1 mm size. Batch adsorption experiments were conducted to assess the influence of initial cadmium concentration, pH of the medium, adsorbent dose and contact time. Subsequently, equilibrium isotherm and kinetic studies were performed using prior optimized conditions. The initial and final concentrations of each adsorption were accurately determined using Inductively Coupled Plasma-Mass Spectrometry. For better accuracy, three replicates were conducted. Optimal cadmium

removal observed at an initial concentration of 0.80 mg/L, achieving 50.63% efficiency. A pH of 7 resulted in the highest efficiency at 30.75%. The most effective biosorbent dose was 0.05 g (33.00%). The optimum contact time was 140 minutes, corresponding to 62.75% removal. Based on equilibrium data, this biosorption process was best fitted with the Freundlich model having a higher regression coefficient (R<sup>2</sup> = 0.9033), confirming a multilayer coverage on the adsorbent. Adsorption capacity of G. quaesita fruit rind is determined to be 1.02 mg/g. Furthermore, kinetic studies show adherence to pseudo- second order kinetics ( $R^2 = 0.9976$ ), suggesting chemisorption as the rate limiting step. This study highlights that G. quaesita can work well as an environmentally friendly material to remove toxic cadmium from aqueous solutions. However, more research is needed to explore how it could also be applied in food-related applications.

## Keywords:

*Garcinia quaesita*; biosorbent; Cadmium removal; adsorption kinetics

## Green synthesis of ZnO nanoparticles using the stem of *Murraya koenigii* and investigation of their photocatalytic activity

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About 20% of the global water pollution caused by the apparel and textile industry is linked to textile dyeing. Chemical dyes used in the production of clothing are often discarded into rivers without proper treatment. These contaminates persist in ecosystems, damaging aquatic life and polluting water sources. To address this issue, the development of eco-friendly and cost-effective solutions is essential. Zinc Oxide (ZnO) nanoparticles (NPs) synthesized through green methods using plant extracts. In photocatalysis, these nanoparticles can act as efficient catalysts. Murraya koenigii, valued for its leaves and berries in culinary and medicinal applications, has an underutilized stem that could potentially offer additional benefits and is explored further in this study. Green-synthesized ZnO nanoparticles were obtained using zinc acetate as the precursor at an optimal concentration of 0.01 mol dm<sup>-3</sup>. The plant extract to precursor ratio was optimized to 1:50, at a pH of 12 and room temperature. The synthesized NPs were characterized using UV-Visible spectroscopy, Fourier Transform Infrared (FTIR) spectrometer, and Scanning Electron Microscope (SEM). The UV-Visible spectrum of synthesized nanoparticles exhibited a distinctive peak at around 360-390 nm, while FTIR analysis showed a peak in the wavenumber range of 500-600 cm<sup>-1</sup>, corresponding to the stretching vibration of Zn-O bonds, confirming the formation of ZnO NPs. SEM analysis revealed that the ZnO NPs had a flake-like morphology, organized in a nano-flower arrangement. The photocatalytic activity of the green synthesized ZnO NPs was evaluated under varying conditions to optimize parameters for dye degradation. The optimum pH was found to be 10, with an optimal ZnO catalytic load of 25 mg and the dye degradation time was optimized to 120 minutes. Under these conditions, the ZnO NPs demonstrated a maximum dye degradation efficiency of 85% for methylene blue (MB) when exposed to solar light. Future studies should focus on exploring antibacterial, antimicrobial, antioxidant potential of green synthesized ZnO NPs. Further investigations are also warranted to elucidate the precise mechanisms of action and to conduct detailed kinetic studies to optimize their efficiency.

#### Keywords:

Green synthesis; *Murraya koenigii*; photocatalytic activity; methylene blue; ZnO nanoparticles

# Evaluation of antibacterial activity in green synthesized chitosan-silver nanoparticles for therapeutic applications

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Green synthesis is a safe and eco-friendly way to make silver nanoparticles. Chitosan, a natural and biodegradable polymer was used as both the reducing and stabilizing agent in the silver nanoparticle synthesis. Chitosan-silver nanoparticles (CS-AgNPs) were synthesized by mixing chitosan (500 mg) with 500 ml silver nitrate solution (2 mM) while heating at 90 °C and stirring for 15 minutes followed by a dropwise addition of sodium hydroxide (1% W/V, 2.50 mL). A visual colour change from pale yellow to reddish brown, along with a surface plasmon resonance (SPR) band by UV-Visible spectroscopy, confirmed CS-AgNPs formation. Synthesized CS-AgNPs were characterized by Transmission Electron Microscopy (TEM), Fourier Transform Infrared Spectroscopy (FTIR). Antibacterial activity of CS-AgNPs was tested against Staphylococcus aureus and Escherichia coli using a liquid broth assay for a two-fold dilution concentration series. UV Visible spectroscopy showed the SPR band at 434 nm, confirming the successful formation of CS-AgNPs. FTIR analysis revealed characteristic bands at 3200-3600 cm<sup>-1</sup> (OH and NH stretching), 1300 and 1000

cm<sup>-1</sup> (C-O stretching) and 1000 to 1250 cm<sup>-1</sup> (CN stretching) indicating the presence of chitosan AgNPs as a capping agent. TEM images showed spherical particles with an average size of 15.68 nm. Optical density (OD600) values of the bacterial cultures were measured after 24h incubation period. Values of CS-AgNPs for the concentration series starting from 250 µg/mL were 0.489, 0.600, 0.773, 1.040, 1.054 respectively for E. coli while for S. aureus values were 0.464, 0.659, 0.732, 0.780, 0.818 respectively for the same concentration series. It was observed that OD600 values were decreased with increasing nanoparticle concentrations. Ciprofloxacin (30 µg/mL) was used as a positive control and OD600 values of 0.059 for E. coli and 0.077 for S. aureus were obtained. These findings demonstrate that CS-AgNPs exhibit dose-dependent antibacterial properties.

### Keywords:

Green synthesis; chitosan; silver nanoparticles; optical density; antibacterial

# Novel curcumin derivatives loaded chitosan nanoparticles as therapeutic agents for alzheimer's disease: an *in-silico* evaluation

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Alzheimer's disease is an irreversible neurodegenerative disorder defined by signs and symptoms that include β-amyloid plaques, tau neurofibrillary tangles, and synaptic dysfunction. Treatments currently available are only palliative, but curcumin has shown promise in the treatment of Alzheimer's disease due to its neuroprotective and anti-inflammatory properties; however, curcumin is limited by low solubility and bioavailability. This study was designed to evaluate novel curcumin derivatives enclosed within chitosan nanoparticles for improved delivery, blood-brain barrier penetration, and therapeutic potential against AD. Six derivatives-bisdemethoxycurcumin, curcumin pyrimidine hybrid, quinolone hybrid, imidazole hybrid, thalidomide hybrid, and di-indole hybridwere selected, their geometries optimized with DFT using Gaussian software, and subjected to molecular docking against key AD-specific proteins: amyloid precursor protein, acetylcholinesterase (AChE), tau protein, amyloid  $\beta$ -a, and amyloid  $\beta$ -a fibrils. Native curcumin and the FDA-approved drug donepezil were used as references. The quinolone hybrid showed the strongest binding to AChE (-9.63 kcal/mol), followed by thalidomide (-9.29 kcal/mol) and di-indole (-9.26 kcal/ mol), outperforming curcumin (-7.43 kcal/mol) and

approaching donepezil (-10.51 kcal/mol). These three compounds also demonstrated favorable interactions with other AD targets, suggesting multitarget potential. To enhance delivery, a chitosan nanoparticle system was evaluated and energy-minimized to simulate a spherical nanocarrier structure. Docking of the nanocarrier with the top three derivatives revealed favorable binding energies of -6.28 kcal/mol (quinolone), -7.37 kcal/ mol (thalidomide), and -6.73 kcal/mol (di-indole), confirming good encapsulation. ADMET and toxicity predictions using ADMETlab 2.0 indicated the quinolone hybrid had the most favorable safety profile, while the others remained within acceptable limits. Overall, the quinolone, thalidomide, and di-indole hybrids are promising anti-Alzheimer agents, with the quinolone derivative showing the best efficacysafety profile. Molecular dynamics simulation of the quinolone hybrid-AChE complex, conducted over 50 ns, demonstrated stable binding interactions, further validating its potential as a lead candidate.

## Keywords:

Acetylcholinesterase; Alzheimer's disease; chitosan nanoparticles; curcumin derivatives; molecular docking

## Development of plasma-activated coconut coir biochar for the efficient removal of rhodamine B, Cu(II), nitrate and ammonium ions from aqueous media

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Access to safe drinking water is a fundamental human right. Developing green, sustainable materials for environmental remediation, particularly water purification, has gained significant momentum in recent years. Carbon-based materials have garnered considerable attention due to their highly tunable surface chemistry. However, conventional methods for synthesizing carbon materials often require high energy input, extensive chemical and solvent consumption, and significantly contribute to the carbon footprint. In this study, we replaced the conventional chemical activation method for carbon surfaces with a nonsophisticated approach using the fourth state of matter. Low-temperature pyrolyzed coconut coir biochar (BC), produced at 500°C, was functionalized using atmospheric air plasma treatment (AAPT) to produce plasma-functionalized biochar (PFBC). Plasma treatment introduced functional groups such as amines, carbonyls, and epoxies, as confirmed by Fourier transform infrared spectroscopy, enhancing the material's adsorption capabilities. Characterization of BC revealed an ash content of (7.7  $\pm$  0.2) % and a moisture content of  $(9.9 \pm 0.5)$  %. The iodine numbers, which indicate microporosity (<2 nm), were (510

 $\pm$  90) mg/g for BC and (570  $\pm$  80) mg/g for PFBC. In comparison, the methylene blue numbers, which indicate mesoporosity (2-50 nm), were  $(47.0 \pm 0.8) \text{ mg/g}$ for BC and (116.0  $\pm$  0.8) mg/g for PFBC. The point of zero charge shifted from  $(7.1 \pm 0.2)$  for BC to  $(8.1 \pm 0.2)$ for PFBC after AAPT. Adsorption studies demonstrated significantly improved pollutant removal efficiencies with PFBC under optimized pH conditions compared to BC. Nitrate removal increased from (6.3  $\pm$  0.4) % to (15.6  $\pm$  0.4) % at pH 2, Rhodamine B from (11.9  $\pm$ 0.3) % to (18.6  $\pm$  0.2) % at pH 10, and ammonium from (16.7±0.6) % to (25.3±0.7) % at pH 8, Cu<sup>2+</sup> from (57.8  $\pm$  0.6) % to (77.3  $\pm$  0.2) % at pH 4. All measurements were performed in triplicate to ensure accuracy and reproducibility. These results demonstrate that plasma activation improves the physicochemical properties of biochar, with the potential to provide a sustainable and efficient approach for removing cationic dyes, heavy metals, and inorganic ions from contaminated water systems.

#### Keywords:

Plasma activation; coconut coir biochar; Rhodamine B; nitrate; ammonium ion; removal

## Effects of bisphenol A and its' substitutes on type 2 diabetes mellitus: an *in-silico* study

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Environmental exposure to endocrine disrupting chemicals (EDCs) like bisphenol A (BPA) is increasingly linked to the development of Type 2 Diabetes Mellitus (T2DM). BPA disrupts glucose regulation and insulin signaling, and its structural analogues and derivatives, introduced as substitutes, show similar biological activity. These compounds interact with nuclear receptors such as Estrogen Related Receptor Gamma (ERRy), a key regulator of energy metabolism, glucose homeostasis and mitochondrial biogenesis, raising concerns about their role in metabolic disorders like T2DM. This study aimed to understand the mechanism of action between BPA and its substitutes under T2DM using in-silico studies, explored through limited research exists and investigates how their binding with metabolic proteins and observe the dynamic structural changes within the receptor-ligand complex. Here the ERRy maintains an active helix conformation and binds endocrine disruptors, revealing molecular interaction details. Ligands bind mainly to helical regions, forming hydrogen bonds with key amino acid residues located within the LBD, disrupting metabolic expression and contributing to insulin resistance and T2DM.Computational studies were performed using DFT with the B3LYP hybrid exchange correlation

function via the basis set 6-31G + (d,p) in aqueous phase, to optimize the geometries of the ligands which are structural analogues of BPA. Bisphenol AP (BPAP), Bisphenol P (BPP), Bisphenol BP (BPBP), Bisphenol G (BPG) and Derivatives which are Tetramethyl bisphenol A (TMBPA), Bisphenol TMC (BPTMC), Dinitro bisphenol A (DNBPA) and Nitro BPA (NBPA). Molecular Docking was performed using Autodock4. Calculated values are based on Low Binding Energies to analyze the bonding interactions between receptorligand complex. Findings revealed that BPTMC exhibited the highest binding affinity with -10.00 kcal/ mol. This has followed by BPP, BPG, BPAP and TMBPA having -8.93 kcal/mol, -8.90 kcal/mol, -8.85 kcal/mol and -8.75 kcal/mol respectively, exhibiting favorable high binding affinities whereas the others were within the expected range. However further molecular dynamic (MD) simulations are required for validating these results. And the bonding interaction analysis focused on identifying Hydrogen bonds between the ligands and active site residues of ERRy receptor.

### Keywords:

BPA, Derivatives, Analogues, Type 2 Diabetes Mellitus, Molecular Docking

## Pomegranate phytochemical-loaded nanocarriers as therapeutic anti-cancer agents: an *in-silico* study

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Melanoma, an aggressive skin cancer arising from abnormalmelanocytes, is often triggered by UV exposure, showing high heterogeneity and poor prognosis due to rapid metastasis. Synthetic BRAF inhibitors such as Vemurafenib, Dabrafenib, and Encorafenib are approved drugs used to treat metastatic melanoma, which causes adverse side effects. Pomegranate (Punica granatum L.) is a natural source offering potent antioxidant, anti-inflammatory, and anti-cancer effects. Its diverse polyphenol content provides stronger free radical scavenging activity, thus mitigating itself as a potential natural anti-cancer therapeutic. Recent research studies have shown that these polyphenols possess strong anti-cancer activity through a variety of mechanisms. An in-silico study can provide insights about these different mechanisms and about structural features required to improve inhibitory activities. In this computational study, sixteen major phytochemicals: Ellagic Acid (EA), Ellagic Acid Glucoside, Ellagic Acid 4-O-xylopiranisode (EAX), Citric acid, 1,3,6,-Tri-O-Galloyl-D-Glucose, D-(+)-Catechin (DC), Gallic Acid, Galloyl-6-O-Diglucoside, Phellatin, Phlorozin, Quercitrin, Vanillic Acid, Cyanidin-3,5-O-Diglucoside, Delphinidin-3-O-Glucoside, Pelargonidin -3,5-O-Diglucoside, Delphinidin-3,5-O-Diglucoside

were subjected to optimization using DFT with B3LYP method and 6-31G basis set and subsequently to molecular docking against the BRAF-V600E protein, which was modeled using SWISS-MODEL. Docking studies were performed using AutoDock 4, where eight phytochemicals showed commendable results with low binding energies where EA (-8.39 kcal/ mol), EAX (-8.26 kcal/mol) and DC (-8.13 kcal/mol) had the lowest. The selected phytochemicals were individually evaluated with chitosan and ovalbuminbased nanoparticle systems, demonstrating promising results in performance and compatibility. However, based on the releasing capability of chitosan, it showed better efficacy. Further, Molecular Dynamic (MD) simulations were conducted to evaluate the stability in physiological conditions. Toxicology studies using ADMET Lab 2.0 revealed that several phytochemicals had favorable safety profiles, while others remained within acceptable limits. Overall, Chitosan was proven in-silico to be a viable nanoparticle drug system with all eligible phytochemicals further being proved through analysis of MD trajectories.

## Keywords:

Chitosan, Docking, Melanoma, Pomegranate



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