CHEMISTRY in Sri Lanka

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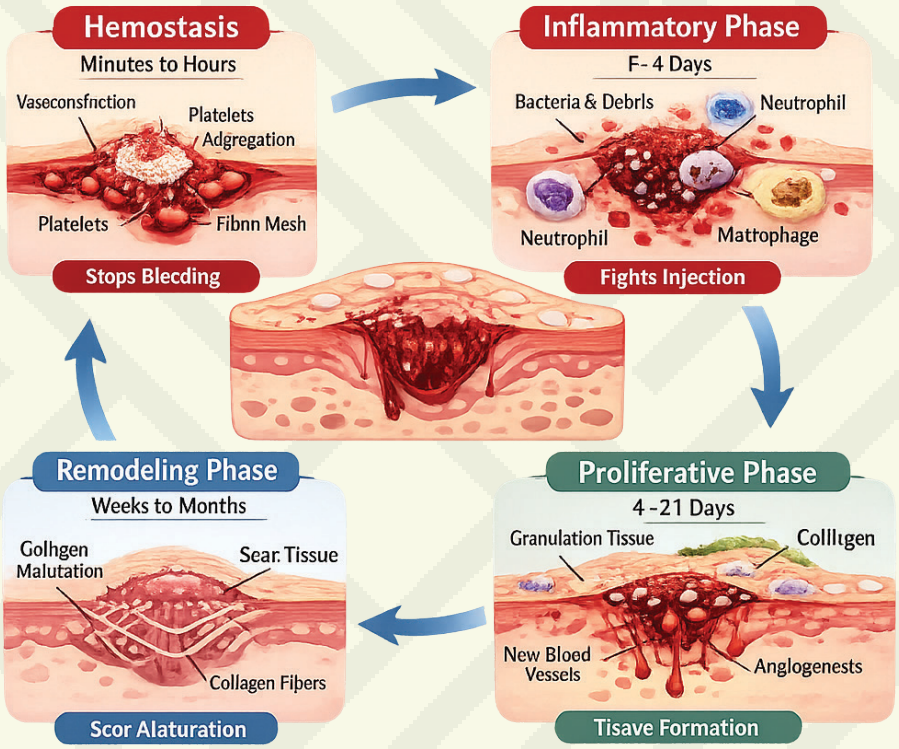
The Phases of Wound Healing



Guest Articles

The Tri Annual Publication of the Institute of Chemistry Ceylon

Chemistry in Sri Lanka ISSN 1012 - 8999

The Tri-Annual Publication of the Institute of Chemistry Ceylon

Founded in 1971, Incorporated by Act of Parliament No. 15 of 1972

Successor to the Chemical Society of Ceylon, founded on 25th January 1941

Vol. 43 No. 1 **January 2026**

Theme for the year -

Journey towards economic sustainability in Sri Lanka - Role of Chemists

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Guest Articles

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

D. Pasindu Dilshan Perera[1], Jayangika Dahanayake[1], Thilomi Samarakoon[2], and Suranga Wickramarachchi[1]

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The rapid rise of nanotechnology has resulted in minute particles, yet powerful such as silver nanoparticles (AgNPs) into countless products, from medical devices to household goods. These metallic specks, celebrated for their potent antimicrobial and catalytic traits, are driving innovation. Yet, as they move from the lab to market, a critical question remains: What happens when these engineered materials enter to environment, especially when they encounter other common pollutants. Recent studies suggest that AgNPs can undergo physicochemical transformations in the presence of other pollutants, such as heavy metals, altering their behavior and toxicity. Cadmium (Cd), a well-known toxic heavy metal, is frequently found in industrial effluents and can co-exist with AgNPs in aquatic habitats. The interaction between these two contaminants can result in synergistic or additive toxic effects, which remain poorly understood. Addressing this knowledge gap requires a multidisciplinary approach that combines material science, computational chemistry, and environmental toxicology.

A major hurdle for using nanoparticles is their inastability?? In water, unprotected AgNPs tend to clump together, which can drastically change their properties and environmental behavior. Our research sought a sustainable solution to address this issue. Chitosan, a natural, renewable polymer derived from crustacean shells. AgNPs were successfully synthesized via a simple, heated reaction. During AgNP synthesis, chitosan plays a dual role: it acts as a green chemical reductant, converting silver ions (Ag^{+}) into metallic silver (Ag^{0}), and, most importantly, as a stabilizing cap to synthesized AgNPs. Chitosan polymer, rich in amine and hydroxyl groups, wraps tightly around the silver, creating a robust shield that prevents the particles from collapsing.

Analytical tests confirmed the formation of the metallic core and secured the presence of the chitosan coating, revealing uniformly dispersed, stable nanospheres. In order to truly validate the effectiveness of the chitosan shield, we moved beyond the physical laboratory into the realm of computational chemistry. This is where Molecular Dynamics (MD) simulations provided atomic-level insights into the system's stability.

To model this accurately the CHARMM force field (Chemistry at Harvard Macromolecular Mechanics) was used with the GROMACS software. A force field is essentially the mathematical blueprint used to calculate the energy and forces acting on every atom in the simulation, allowing us to predict their movement over time. In the CHARMM model, the total energy of the system is the sum of bonded interactions (like the spring-like forces holding the chitosan molecule together) and non-bonded interactions (like the attractions and repulsions between different molecules). The non-bonded terms, which include van der Waals forces and electrostatic forces (based on atomic charges), are critical for modeling the securing interaction between the chitosan and the silver surface.

The MD simulations, powered by this precise force field, confirmed that the CS-AgNPs remained structurally sound and highly stable over the entire simulation period. This demonstrated that the non-covalent, hydrogen-bonding forces exerted by the chitosan are highly effective in maintaining

the nanoparticle's integrity in an aqueous setting, reinforcing the synthesis success computationally.

The final, and most crucial, step was to test the environmental impact of AgNPs when released to water bodies. *Moina macrocopa*, a common freshwater crustacean was chosen as the model organism for *in-vivo* toxicity assessment. The individual effects of CS-AgNPs and heavy metal toxin Cadmium (Cd), and their combined presence on *Moina macrocopa* were assessed.

As anticipated, CS-AgNPs exhibited only mild toxicity to *Moina macrocopa*, suggesting the protective polymer coating was effective. Cadmium, a well-known pollutant, caused significant harm even at low concentrations. However, the results from the combined exposure were alarming: the toxicity was synergistic. The organisms suffered a far steeper decline in survival, growth, and reproduction when exposed to both contaminants than would be expected from simply adding their individual effects. This synergistic effect suggests that the chitosan, while stabilizing the silver core, might also be complexing with the cadmium ions. This new interaction could potentially enhance the uptake of the highly toxic metal species by the *Moina macrocopa*, highlighting a hidden hazard in complex aquatic systems.

This research stands as a powerful demonstration of the need to merge experimental chemistry with advanced computational prediction. We have successfully proven that chitosan is an excellent green stabilizer for silver nanoparticles. However, the discovery of enhanced toxicity in the presence of cadmium serves as a vital environmental warning.

Moving forward, the development of nanotechnology must be guided by this holistic approach. We must evaluate nanomaterials not in isolated, pristine laboratory conditions, but under environmentally realistic scenario where interactions with co-existing pollutants like heavy metals are the norm. This work provides a robust framework, accelerating the rational design of future materials that balance high performance with necessary environmental safety.

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Prevulcanization of Natural Rubber Latex

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Natural rubber latex is the sap of the *Hevea brasiliensis* which is commonly known as the rubber tree or Pará rubber. It is a colloidal dispersion of *cis*-1,4-polyisoprene particles in water and is an important polymeric raw material for manufacturing both latex-based products and dry rubber products, such as gloves, balloons, mattresses, and tires. Traditional vulcanization of rubber mainly refers to the vulcanization of dry rubber, which occurs after molding and shaping, where heat and chemical additives induce crosslinking in the solid state. Prevulcanization, by contrast, involves the controlled formation of crosslinks while the rubber remains in its latex stage, without disturbing its colloidal stability. This an important modified latex-based raw material offers significant advantages in process efficiency, energy consumption, and control over final material properties, especially for latex-based products such as gloves.

Pervulcalization:

Prevulcanized natural rubber latex is defined as modified latex grade in which the dispersed rubber particles undergo partial chemical crosslinking while retaining their fluidity and colloidal stability. This early-stage crosslinking is typically achieved by the addition of sulphur, accelerators, activator and other compounding agents. Importantly, the latex maintains its original dispersion characteristics, enabling storage, transport, and processing similar to unvulcanized latex. Commercial centrifuged natural rubber latex can be vulcanized using sulphur curing system, peroxide system, or high-energy radiation such as gamma-ray or electron beam irradiation. Among the methods sulphur prevulcanized latex is still the dominant industry accepted method to date.

Sulphur prevulcanization

In this process, natural rubber latex is first stabilized with a surfactant such as Sodium dodecyl sulfate (SDS) and KOH to maintain the colloidal stability of the latex during the reaction. Then the latex is compounded with sulphur, accelerators, activators such as zinc oxide, and other necessary ingredients, allowing controlled crosslinking to occur within the dispersed rubber particles. Commonly for the prevulcanization ultra-fast accelerators such as Zinc 2-Mercaptobenzothiazole (ZMBT), zinc-dibutyldithiocarbamate (ZDBC), Zinc Diethyldithiocarbamate (ZDEC) are used. During the prevulcanization process, sulphur crosslinks are formed within the rubber particles as shown in figure 1.

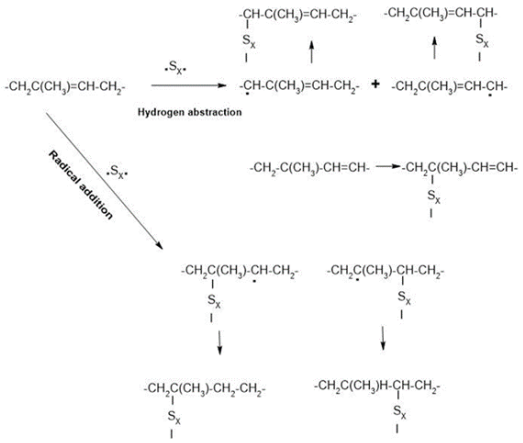

Figure 1: Two proposed mechanisms for sulphur pre vulcanization.

A study by Tangboriboonrat et al. (2002) demonstrated that a homogeneous network of sulphur-crosslinked isoprene chains develops within each rubber particle, independent of particle size. In this system, the vulcanizing agent (sulphur) dissolves in the rubber phase more rapidly than in peroxide-initiated systems. By adjusting the ratio of sulphur to accelerators, it is possible to form mono-, di-, or polysulfidic linkages, enabling the production of prevulcanized latex with varying moduli and mechanical properties. This flexibility allows the formulation of latex suitable for a wide range of applications, from soft, flexible films to high-modulus dipping products.

The degree of crosslinking achieved during prevulcanization has a profound effect on film formation and mechanical properties. Highly crosslinked particle

surfaces restrict chain mobility, impairing particle coalescence and producing weak films. Conversely, homogeneous crosslinking within the latex particles promotes uniform fusion during film formation, resulting in films with superior tensile strength, elasticity, and tear resistance. Hence, controlling the extent of prevulcanization is critical for ensuring reproducible product performance. The degree of crosslinking is usually measured using equilibrium-swelling test (in toluene), Modulus test or estimated via Chloroform coagulation test.

Peroxide Vulcanization

Peroxide vulcanization is an alternative crosslinking mechanism, where thermal decomposition of organic peroxides generates free radicals that induce carbon–carbon crosslinks as shown in figure 2. Peroxide-vulcanized latex exhibits high thermal stability and low compression set, rendering it suitable for specialized applications. Nevertheless, peroxide systems are less prevalent industrially due to higher material costs, handling considerations, and generally lower tensile strength compared to sulphur-based systems.

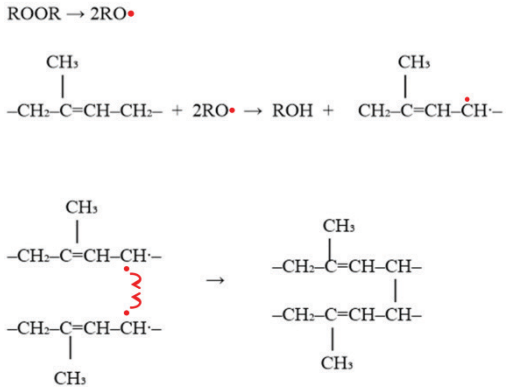

Figure 2: Reaction mechanism of peroxide curing.

Radiation Vulcanization

Radiation vulcanization employs high-energy ionizing radiation, such as γ-rays or electron beams, to induce crosslinking in latex. Free radicals generated within the rubber macromolecules lead to crosslinks without requiring elevated temperatures or chemical accelerators. γ-radiation, commonly sourced from Cobalt-60, is preferred for its high penetration power, whereas Caesium-137, despite a longer half-life, is rarely used due to lower γ-energy.

Electron beam irradiation has emerged as a controllable alternative, allowing precise adjustment of crosslink density. Low to moderate doses enhance mechanical properties, including modulus, tensile strength, elongation at break, and tear resistance. Excessive doses can cause chain scission and degradation, highlighting the importance of dose optimization. Transmission electron microscopy studies have confirmed that radiation vulcanization produces relatively homogeneous crosslinking within latex particles, favoring film formation and mechanical performance.

Radiation vulcanization offers several advantages: reduced chemical usage, room-temperature processing, and formation of carbon–carbon crosslinks with superior thermal stability. These characteristics are particularly advantageous for latex-based products subject to strict regulatory constraints, such as nitrosamine limits, accelerator- and protein-induced allergies, zinc discharge control, and environmental considerations during disposal. Despite these benefits, high capital and operational costs, coupled with safety and regulatory requirements, have limited widespread industrial adoption.

Industrial Applications and Advantages

Prevulcanized latex is ideally suited for dipping applications, such as gloves, condoms, and elastic coatings. Sulphur-based prevulcanization remains the preferred industrial route due to its cost-effectiveness, reproducibility, and scalability. Radiation and peroxide methods provide alternatives for high-performance or regulatory-sensitive applications, offering cleaner, chemically stable, and mechanically robust latex.

Overall, the prevulcanization of natural rubber latex represents a critical strategy in modern rubber technology. By precisely controlling crosslinking at the

particle level and optimizing maturation conditions, manufacturers can produce latex products with tailored mechanical properties, enhanced stability, and compliance with environmental and health regulations.

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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 May 2026.

- *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.

Guest Articles

The Chemistry of Bacterial Exopolysaccharides

Indushika Anjanee & Duleepa Pathiraja
Department of Chemistry, University of Colombo

Introduction

Bacteria synthesize a wide range of biopolymers with unique chemical structures, utilizing simple and complex substrates. Depending on their location within the cell, these biopolymers can be classified as either intracellular or extracellular. Extracellular biopolymers, often called Exopolysaccharides (EPSs), are more diverse and essential for bacterial survival and adaptation than intracellular biopolymers, which are comparatively fewer in number and function.[1] Bacterial EPSs have clear advantages over plant, animal, and algae-derived polysaccharides because they can be produced year-round under controlled fermentation conditions, are easily and cost-effectively recovered from cell-free culture supernatants, and allow tunable yields and polymer properties through genetic or metabolic engineering.[2] Their biological functions are pivotal: EPSs provide physical protection against desiccation, toxic compounds, antibiotics, and phagocytosis, while also mediating adhesion to surfaces and cell-to-cell communication.[1,2] The vast chemical and structural variety inherent to bacterial EPSs, coupled with the precision of microbial fermentation, allows for the tailored production of biopolymers with exceptional and predictable functional properties, positioning them as cornerstones in the modern food, pharmaceutical, and bioremediation sectors. This article focuses on the chemical characteristics that underlie this versatility, highlighting a clear link between their molecular structure and its macroscopic utility.

Structural Architecture and Classification

Bacterial EPSs display remarkable chemical diversity, reflecting the wide range of biological roles they perform. At the molecular level, their architecture is defined by several key parameters, including monosaccharide composition, molecular weight, glycosidic linkages, functional groups, branching patterns, and higher-order microstructure.[3]

The most fundamental distinction arises from the primary structure, specifically the nature of the constituent sugar units. On this basis, EPS are broadly categorized as homopolysaccharides (HoPSs), composed of a single type of monosaccharide, or heteropolysaccharides (HePSs), which contain two or more different monosaccharide residues arranged in repeating units. HoPSs include structurally simpler polymers such as curdlan, while HePSs often consist of repeating oligosaccharide blocks ranging from disaccharides to heptasaccharides, resulting in greater structural complexity.[1,4] Common monosaccharides such as glucose, galactose, and fructose are frequently encountered, but many EPS also incorporate rarer sugars like rhamnose, fucose, xylose, and mannose, as well as uronic acids and amino sugars, contributing to their functional versatility.[4]

In addition to monosaccharide composition, EPSs are further classified according to the glycosidic linkages that join individual sugar units. These bonds are defined by the carbon atoms involved, most commonly C1–C3, C1–C4, or C1–C6, and by their α or β configuration.3 In the polymer backbone, β-(1→4) and β-(1→3) linkages generally produce more rigid structures, whereas α-(1→2) and α-(1→6) linkages result in greater chain flexibility.[1] These bonding patterns strongly influence the overall shape of the EPS molecule. Polysaccharides with straight, unbranched chains, such as pullulan, are classified as linear EPS, while those containing side chains and bends, such as EPS-W1 from *Lactobacillus plantarum* W1, are referred to as branched EPS.[4] Additional chemical features, including the presence of neutral or charged functional groups and non-carbohydrate substituents such as phosphate, acetyl, or glycerol moieties, further expand the classification framework by imparting ionic character and altering physicochemical behavior.

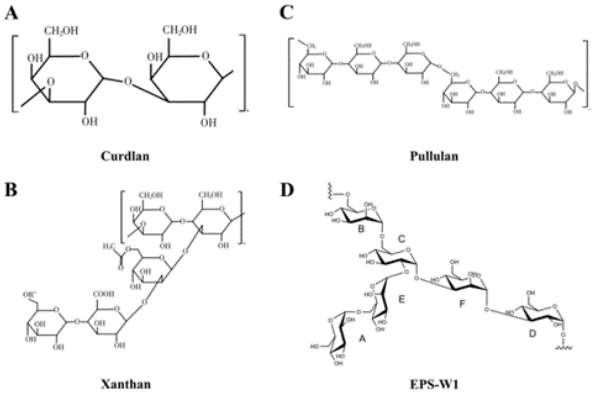

Figure 1: EPS structure of homopolysaccharides [e.g., curdlan (A)]; heteropolysaccharides [e.g., xanthan (B)]; linear polysaccharides [e.g., pullulan (C)]; and branched polysaccharides [e.g., EPS-W1 (D)].[4]

Chemical Modification of EPS

Chemical modification of EPSs has gained increasing attention as a means to tailor their molecular structure and enhance targeted biological functions. These modifications are achieved by introducing functional groups onto the polysaccharide backbone.[4] Carboxymethylation introduces carboxymethyl groups through etherification reactions, increasing water solubility and improving biological performance.[5] For example, carboxymethylated EPSs from *Lachnum* fermentation broths significantly reduced fasting blood glucose and serum triglyceride levels while improving insulin sensitivity in diabetic mouse models, highlighting their potential use in functional foods and therapeutic formulations.[6] Acetylation modifies the steric configuration of EPS by adding acetyl groups, which have been shown to improve reducing power and antioxidant capacity.[7] Phosphorylation is another effective modification strategy, introducing phosphate groups that increase negative charge density and strengthen biological interactions. Phosphorylated EPS from *Lactococcus lactis* and Lachnum species demonstrated significantly improved antioxidant activity both in vitro and in vivo, indicating potential applications in nutraceuticals and biomedical materials. Similarly, sulfonation improves solubility and chain flexibility, resulting in stronger antioxidant and antimicrobial effects, as observed in EPSs from *Enterobacter cloacae* and *Streptococcus thermophilus*.

The Chemistry of EPS Biosynthesis

In bacteria, EPSs are produced through four principal pathways.8 In all intracellular pathways, EPS biosynthesis relies on a common chemical principle: the generation of activated sugar precursors, followed by enzyme-catalyzed glycosyl transfer reactions that construct the polymer backbone and its substituents.

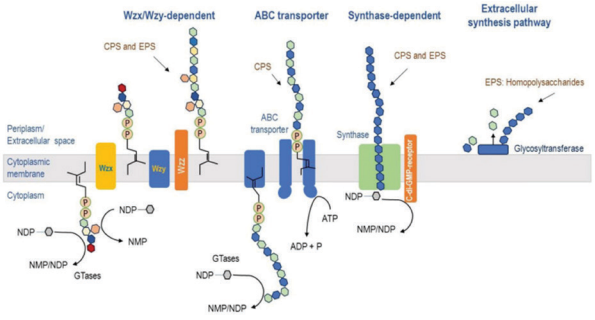

Figure 2: Biosynthesis of polysaccharides in microorganisms.[8]

The chemical foundation of EPS biosynthesis lies in the formation of sugar nucleotides, which act as high-energy donors for glycosylation reactions.[9] Simple sugars derived from central metabolism, such as glucose-6-phosphate or fructose-6-phosphate, are enzymatically converted into sugar-1-phosphates and subsequently activated through reactions with nucleoside triphosphates, typically UTP, GTP, or TTP. This process yields sugar nucleotides such as UDP-glucose, UDP-galactose, UDP-glucuronic acid, GDP-mannose, and TDP-rhamnose.[8] The cleavage of the phosphodiester bond during glycosyl transfer provides the thermodynamic driving force for forming new glycosidic linkages.[10] The nucleotide moiety also serves as a molecular recognition tag, ensuring that each glycosyltransferase incorporates the correct monosaccharide at the appropriate position, thereby preserving the fidelity of EPS structure.

Among EPS biosynthetic routes, the Wzx/Wzy-dependent pathway is the most chemically complex and mainly produces HePSs. Repeating oligosaccharide units are assembled on the cytoplasmic face of the inner membrane on undecaprenyl phosphate (a C55 isoprenoid lipid acts as a mobile chemical carrier), modified by specific glycosyltransferases, flipped across the membrane by Wzx, and polymerized in the periplasm by Wzy to yield high-molecular-weight EPSs

such as xanthan.[8] In contrast, the ABC transporter–dependent pathway, primarily associated with capsular polysaccharide (CPS) biosynthesis, exports completed polymers through an ABC transporter and generates CPSs with a glycolipid terminus containing phosphatidylglycerol and a poly-keto-deoxyoctulosonic acid (Kdo) linker, which anchors the polysaccharide to the cell envelope.[11] The synthase-dependent pathway is a simpler strategy in which polymerization and secretion occur simultaneously through a single synthase enzyme or complex.[12] This pathway mainly produces HoPSs such as cellulose, curdlan, alginate, and hyaluronic acid, where activated sugar nucleotides are directly added to the growing chain as it is extruded across the membrane.[8] While some polymers, like cellulose and curdlan, consist of a single type of sugar and linkage, others, such as alginate, are further diversified by post-polymerization modifications, such as alginate which is first synthesized as polymannuronic acid and later modified by epimerases to generate varying mannuronic and guluronic acid sequences.[13] In contrast, some EPSs are synthesized entirely outside the cell by secreted glycosyltransferases that use substrates like sucrose, producing polymers such as dextran and levan. This extracellular mechanism bypasses sugar nucleotides and membrane carriers, representing a distinct chemical route to EPS formation.

The Rheological Chemistry

Many EPS contain uronic acids (such as glucuronic and galacturonic acid) and pyruvate ketals, which introduce carboxyl groups into the polymer backbone.[14] At neutral pH, these groups are ionized, making EPS highly polyanionic molecules. The resulting negative charge density causes the polymer chains to adopt extended conformations and promotes strong interactions with water through electrostatic forces and hydrogen bonding. This explains the high hydration capacity of EPS and their ability to form viscous solutions even at low concentrations. In addition, the negatively charged sites readily bind metal ions such as Ca^{2+} and Mg^{2+}, a property that contributes to biofilm stability and is widely used in food stabilization and water treatment.[15]

EPS are mostly high-molecular-weight polymers, often ranging from 10^5 to over 10^7 Da. Their large size leads to significant chain overlap and physical entanglement in solution, which results in high viscosity. Their large size leads to extensive chain overlap and physical entanglement in solution, producing high viscosity. Unlike simple liquids, EPSs solutions usually show non-Newtonian flow behavior, where viscosity decreases with increasing shear stress. This shear-thinning behavior is especially evident in HePSs such as xanthan. Xanthan adopts an ordered double-helical structure in solution, forming a weak but extensive network at rest that results in high viscosity and yield stress. Under shear, the helices align with the direction of flow and temporarily disentangle, causing a reversible drop in viscosity. When shear is removed, the original structure rapidly reforms, allowing viscosity to recover.[16] Xanthan's rheological behavior is further influenced by acylation and salt concentration: pyruvate groups stabilize the ordered structure, while acetyl groups tend to destabilize it and reduce synergistic gel formation.[17]

In contrast to xanthan, dextrans form aqueous solutions that behave largely as Newtonian fluids, with viscosity dependent on concentration, temperature, and molecular weight.[18] Native dextrans are polydisperse, with molecular masses typically ranging from 10^6 to 10^9 Da. Controlled acid hydrolysis produces fractions with defined molecular weights, a property that, combined with their low immunogenicity, has enabled widespread clinical and pharmaceutical use, including as blood plasma expanders and chromatography matrices.[15]

Some EPSs also undergo gel formation through specific molecular associations. In polysaccharides such as curdlan and gellan, gelation occurs when polymer chains transition from flexible random coils to ordered helical structures that aggregate into stable junction zones; this process is often thermoreversible.[19] In contrast, gelation in alginate is driven by ionic interactions rather than temperature. Alginate chains contain guluronic acid-rich regions that selectively bind divalent cations, particularly Ca^{2+}, forming strong ionic cross-links between adjacent chains via the well-known "Egg-Box" mechanism.[20] The resulting hydrogels are mechanically stable and widely used in food, pharmaceutical, and biomedical applications.

Engineered Chemistry and Future Outlook

The functional versatility of bacterial EPSs is closely linked to their finely controlled chemical architecture. Unlike many plant-derived polysaccharides, EPS possess highly regular repeating units, variable molecular weights, and chemically active substituents such as uronic acids, acetyl groups, and pyruvate residues. Due to these features, EPS have found widespread use in food systems, pharmaceuticals, cosmetics, and environmental applications. For example, EPS produced by probiotic Lactobacillus species contributes not only to desirable texture in fermented dairy products but also supports beneficial health effects such as immune regulation, reduction of cholesterol levels, and possible antitumor activity.[1] Similarly, bacterial EPS emerge as safe and biodegradable alternatives to synthetic flocculants in water and wastewater treatment, where they effectively aggregate suspended particles without the health risks associated with aluminium salts or synthetic polymers.[1]

Looking ahead, advances in bioengineering and synthetic biology are transforming EPS production from a largely natural process into a tunable chemical platform. By modifying genes involved in EPS biosynthesis, such as glycosyltransferases, epimerases, and acetyltransferases, researchers can tailor monomer composition, chain length, and degree of substitution to achieve desired material properties. Emerging strategies, including domain swapping of biosynthetic enzymes and the design of synthetic gene clusters, offer the possibility of producing entirely new EPS structures with novel functions. As understanding of structure–function relationships deepens, engineered bacterial EPSs are expected to play a central role in developing sustainable biomaterials for healthcare, environmental remediation, and next-generation biotechnological applications.

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Cover Page

The cover page graphic illustrates the four main phases of wound healing: hemostasis, inflammation, proliferation, and remodeling. It shows how the body first stops bleeding, then removes bacteria and damaged tissue, builds new tissue and blood vessels, and finally strengthens the repaired area to form mature scar tissue. In relation to the guest article titled "Chemical Mediators of Inflammation: Targets for Wound Repair," the diagram highlights the importance of inflammatory mediators in coordinating each stage of healing and influencing successful tissue repair.

(see pages 16 - 20)

Transition-State-Guided Strategies in Natural Product-Based Drug Design

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For over a century, natural products have played a pivotal role in modern medicine, serving as sources of essential drugs for the treatment of infectious, oncological, metabolic, and neurological disorders. These compounds have evolved in plants, microbes, and animals to interact specifically with biological targets, resulting in complex structures and diverse chemical features that confer biological relevance.[1] One notable example is the recent approval of eribulin mesylate, a synthetic derivative of the marine natural product halichondrin B, which has shown efficacy in treating metastatic breast cancer.[2] Nevertheless, developing effective drugs from natural products remains a slow and challenging process, primarily because biological systems are inherently complex and dynamic, and these complexities are not fully addressed by conventional screening methods.[3]

In the past three decades, molecular simulation has become essential for elucidating molecular behavior at the atomic scale. Molecular dynamics simulations enable the observation of proteins, nucleic acids, and ligands over time, capturing critical fluctuations, conformational changes, binding events, and reactions that are fundamental to biological function. Unlike static models, which only provide a snapshot in time, molecular dynamics reveals the temporal evolution of molecular interactions, highlighting dynamic phenomena that static models miss. It is now widely accepted that processes such as enzyme catalysis, ligand recognition, and allosteric regulation are intrinsically dynamic and cannot be fully understood through static structural analysis alone.[4] Despite significant advances in molecular dynamics methodologies, broader adoption in biological and pharmaceutical research is hindered by challenges in simulation setup, software heterogeneity, and the lack of standardized, reproducible computational environments.

To overcome these obstacles, researchers developed the Biomolecular Reaction and Interaction Dynamics Global Environment (BRIDGE)[5, 6], an open simulation platform built on the Galaxy framework. BRIDGE integrates genomics, bioinformatics, and molecular simulation within a unified system. It provides web-based tools for configuring, executing, and analyzing molecular dynamics simulations, along with advanced capabilities for interpreting simulation outcomes.

Although classical molecular dynamics is valuable for investigating binding events and conformational changes, numerous biological processes also involve chemical reactions that form or break covalent bonds. Accurate modeling of these reactions requires hybrid quantum mechanics/molecular mechanics (QM/MM) approaches, in which the reactive region is treated quantum-mechanically, and the remainder of the system is modeled classically. In contrast, purely quantum mechanical (QM) methods offer higher accuracy by treating the entire system quantum-mechanically, but they are often computationally infeasible for large biological systems due to intensive resource requirements. Therefore, QM/MM provides a practical balance between accuracy and tractability. QM/MM has become a standard methodology for elucidating enzyme function, enabling the calculation of reaction energy profiles, transition states, and the roles of specific amino acid residues. A recently developed method, the Free Energies from Additive Reaction Coordinate Forces (FEARCF) method, has provided a detailed framework for decomposing reaction energies and elucidating the factors underlying catalytic efficiency.[7, 8]

The FEARCF method enables researchers to characterize reaction pathways from QM/MM simulations by projecting forces onto the reaction coordinate. This approach quantifies the contributions of specific interactions, electrostatic effects, and protein dynamics to the stabilization or destabilization of the transition state. Such insights extend beyond simple estimates of energy barriers by elucidating their magnitudes and underlying causes, as well as by identifying strategies to modulate them. This concept aligns with Linus Pauling's transition-state hypothesis in enzymology and drug design, which posits that enzymes achieve catalytic efficiency by binding the

transition state more tightly than the substrate, thereby reducing the activation energy and accelerating the reaction.[9, 10] As a result, the design of molecules that mimic the transition state can produce highly potent enzyme inhibitors.

One primary approach is to design transition-state analogues at the atomic level. Once the geometry, charge distribution, and key interactions of a transition state are defined, researchers can synthesize molecules that closely replicate these features. This approach has yielded some of the most potent enzyme inhibitors to date. However, such analogues are often highly complex, strained, or contain unusual functional groups, rendering their synthesis and large-scale production challenging. As the structural fidelity to the true transition state increases, synthetic difficulty also rises, necessitating a balance between molecular accuracy and practical manufacturability.to identify transition-state mimics in existing chemical collections, particularly among natural products. Evolution has created a wide variety of molecules, and traditional medicine has often found active compounds even when their exact effects were unknown. By screening natural product databases with templates based on transition-state shape and charge, researchers can find molecules that resemble the key configuration of a target enzyme. This method avoids many problems of designing new molecules from scratch and combines practical experience with detailed scientific understanding to help discover new, mechanism-based drugs.[11]

This strategy is most effective when supported by computational platforms that integrate molecular databases, simulation tools, reaction modeling, and statistical analysis within a unified workflow. Open platforms such as BRIDGE are well-suited to this purpose, as they integrate simulation engines, analytical tools, and reaction modules into reproducible workflows. This configuration enables transition-state calculations, molecular docking, molecular dynamics, and energy analyses within workflows that can be shared and refined by the scientific community. Consequently, open computational systems are transforming molecular simulation into a more scalable and collaborative discipline.

Natural products are well-suited to this computational approach. Their complex structures and diverse features often make them more similar to enzyme transition states than simple synthetic molecules. By using transition states from QM/MM simulations as search templates, researchers can find natural molecules that might mimic the key conformations of certain enzymes. After identifying these candidates, scientists can use docking and molecular dynamics simulations to assess binding affinity, complex stability, and how protein motion affects binding.

The integration of natural product chemistry, transition-state theory, and open molecular simulation represents a significant advancement in drug discovery. Rather than relying on empirical screening, this approach utilizes mechanistically informed templates based on the functional characteristics of target enzymes. Transparent, reproducible workflows supplant ambiguous procedures, directly linking biological data to detailed molecular insights. Natural products are increasingly recognized as components of an extensive, evolutionarily shaped chemical library accessible to modern computational chemistry, rather than as isolated curiosities. To bridge the gap between computational predictions and real-world applications, experimental follow-up is crucial. This involves validating computational predictions through targeted in vitro and in vivo experiments to ensure that predicted interactions are observed in biological systems. Such experimental validation enhances the reliability of computational models, thereby reinforcing their role in the full research pipeline.

As chemistry enters an era defined by data-driven, simulation-guided discovery, the integration of biodiversity, quantum mechanics, and open computational infrastructure is becoming increasingly essential. Platforms such as BRIDGE exemplify the potential to unify genomic data, protein structures, molecular dynamics, and reaction chemistry within a single framework. Innovations such as FEARCF further facilitate quantitative analysis of the most complex aspects of enzyme catalysis, particularly transition states. Collectively, these advances are reshaping chemists' and biologists' perspectives on molecules, mechanisms, and therapeutics, thereby supporting the shift from natural molecular diversity to rational, transition-state-guided drug discovery to address urgent health challenges.

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Chemical Mediators of Inflammation: Targets for Wound Repair

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Introduction

The ability of fighting infection, healing damages and the capability of energy storage for low nutrient obtainable and high energy need periods, aid the survival of a multicellular organism (Wellen and Hotamisligil, 2005). Healing can be defined as the attempt of the body to restore its regular structure and functions in response to an injury (Sarabahi and Tiwari, 2012). Wound is a constrained injury which is caused by external factor and it can involve any tissue and organ. Wound healing is a compound and sophisticated procedure, comprises a set of events that involve cellular and molecular interaction to restore function of the affected site (Ameh et al., 2020). Wound healing occurs in four main phases including inflammation phase (Stroncek and Reichert, 2008).

Defense mechanism of the body consists of an important part known as inflammation. This is when the healing process initiates by the immune system recognizing any harmful or foreign stimuli in the body (Pahwa et al., 2020). It is also defined as "the body's immune system's response to stimulus" by US National Library of Medicine (Bhatia et al., 2015).

The mechanism of inflammation will be facilitated by several chemical substances and signaling molecules, secreted by the defensive cells of the body (Abdulkhaleq et al., 2018). These soluble and diffusible substances are recognized as chemical mediators which are crucial in inflammatory response, hence in wound healing (Edwards, 2014).

Exploration of therapeutic target is the base of modern drug discovery. The ongoing studies have led to a growing interest in inventing new targets and more exploration of existing targets (Zheng et al., 2006). The chemical mediators are one of the known therapeutic targets in the instance of healing wounds.

This review mainly focuses on the processes of inflammation and wound healing. In addition, this will also focus on how chemical mediators facilitate inflammation while acting as the therapeutic target of wound healing.

Chemical mediators and their types

Chemical mediators can be found in the body tissues; therefore, they are also known as endogenous or permeability factors (Oliviero and Scanu, 2017). While inflammatory response initiated by an injury, the chemical mediators secreted by plasma, cells or tissues in the injured site mediate the process (Anderson and Cramer, 2015).

According to the derivation sites of the mediator molecules, they are classified into two main groups;

1. Cell derived mediators, which are produced by the cells at inflammation site.
2. Plasma derived mediators, which are generally synthesized by the liver and can be found in the plasma as inactive precursors until inflammation occurs.

Different types of chemical mediators perform various functions in the case of inflammation. The table 1 below shows various actions of inflammation occurred due to by different chemical mediators.

Use of chemical mediators in the process of inflammation

Inflammation process

Inflammation is one of the vital processes required in defense mechanism of cells against injuries and infections (Nathan and Ding, 2010). The process of inflammation represents a chain of organized and dynamic responses consisting of cellular as well as vascular events with specific secretions known as chemical mediators (Akcay, Nguyen and Edelstein, 2009). The inflammatory response may consist of

Table 1: Actions of different types of mediators in inflammation

Type of Chemical Mediator	Mediator	Principal Source	Actions
Cell-Derived Mediators	Histamine	Mast cells, basophils, platelets	vasodilation, increased vascular permeability, endothelial activation
	Serotonin	Platelets	vasodilation, increased vascular permeability
	Prostaglandin	Mast cells, Leukocytes	vasodilation, pain, fever
	Leukotrienes	Mast cells, Leukocytes	increased vascular permeability, chemotaxis, leukobyte adhesion and activation
	Platelet-activating factor	Mast cells, Leukocytes	vasodilation, increased vascular permeability, leukocyte adhesioin, chemotaxis, degranulation, oxidative burst
Plasma-Derived Mediators	Complement products (C5a, C3a, C4a)	Plasma (produced in the liver)	Leukocyte chemotaxis and activation, vasodilation (mast cell stimulation), increased vascular permeability, smooth muscle contraction, vasodilation, pain, endothelial activation, leukocyte recruitment
	Kinins		
	Proteases activated during coagulation		

several crucial events; Table 2 explains the use of chemical mediators in various inflammatory responses.

Table 2: Chemical mediators in Different Inflammatory responses.

Inflammatory Response	Chemical mediator
Increased vascular permiability	Vasoactive amines, Bradykinin, Leucotrienes
Fever	IL-1, TNF, Prostaglandins
Pain	Prostaglandins, Bradykinin
Tissue Damage	Neutrophil and macrophage, lysosomal enzymes,
Vasolidation	Prostaglandins, histamine, nitric oxide
Chemotaxis, leukocyte recruitment and activation	Leucotriene, chemokines, Bacterial products

The pathway involves migration of plasma, several white blood cells including monocytes, basophils, neutrophils and eosinophils in the inflammation site (Pober and Sessa, 2007). The mediators and several signaling molecules will be released by the immune defense cells to contribute in the process of inflammation.

The indicators of inflammatory response can be divided as macroscopic and microscopic indicators. The Roman Physician, Celcius explained that macroscopic indicators typically categorized by four "Cardinal Signs" which may give rise to loss of function in the organism (Lotze and Thomson, 2005). Figure 1 illustrates the four cardinal signs.

Figure 1: Cardinal Signs of Inflammation

The inflammatory response may trigger through two phases, which are mediated through different mechanisms.

The immune responses which are involved in acute inflammation can be divided into vascular and cellular processes (Sattar et al., 2009). The responses occuring in microvasculature, commonly appear immediately following the injury or infection in the presence of vascular events known as inflammatory stimuli. These rapid processes sooner will lead to vasodilation and later makes the vessels additionally permeable. This will allow the inflammatory mediators to enter and

contribute to interstitial edema.

Etiology of inflammation

Inflammation may be a result of several factors including physical, chemical and biological agents (Siraj, 2020). Factors such as inappropriate immunological responses, tissue death, infectious agents also trigger inflammation.

Microbial infections are most common cause of inflammation. They give rise to inflammation by entering and destroying cellular components or even cells of the body. Bacteria can secrete a chemical substance known as endotoxins, which can initiate inflammation. Moreover, physical factors such as burn, radiation, injuries, corrosive chemicals and frostbites can also induce inflammation by tissue damage. Inflammation process can also take place when a tissue dies from lack of nutrients and oxygen, which can happen when the blood flow to the tissue is blocked (Nathanael et al., 2011). Apart from these exogenous causes, there are few endogenous factors which can also result in inflammation. Examples for some endogenous factors are; circulatory disorders, activation of several enzymes such as acute pancreatitis, metabolic products such as uric acid (Srikrishna and Freeze, 2009). Figure 2 below shows some of the causes of inflammation.

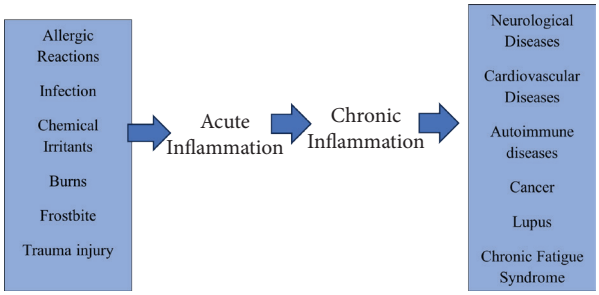

Figure 2: Etiology and cause of inflammation.

Chemical mediators as therapeutic target in progression of wound healing

Process of wound healing

Consequent to tissue damage or injury, a set of events occur in the body. That include inflammation, proliferation and maturation which promote wound closure and restoring of the tissue (Shukla et al., 2019).

The mechanism of wound healing involves two distinct processes; regeneration and repair. They consist of a series of cellular and molecular actions which arise after the onset of a tissue abrasion to restore the injured tissue (Gonzalez et al., 2016). The process of proliferation of parenchymal cells occur during regeneration. Usually, regeneration of tissue results in a complete restoration of the original tissue (Koria, 2012).

The proliferation of connective tissue rudiments resulting in scarring and fibrosis is referred to as tissue repair. This includes granulation of tissue formation and contraction of the wound. Several cells are involved in the repair mechanism, such as; mesenchymal cells, macrophages, endothelial cells and platelets (Neuss et al., 2009).

The initial stage of wound healing is dedicated to hemostasis and the development of a temporary wound matrix, which happens instantly after injury and completed after several hours (Rosinczuk et al., 2018). Additionally, homeostasis will initiate the inflammatory process. Inflammation becomes activated during the phase of coagulation and may approximately get divided into an early stage with neutrophil cell recruitment and late stage with the appearance and alteration of monocytes (Shukla et al., 2019).

The recovery of the wound surface is the main target of proliferation stage. The granulation tissue formation and vascular network restoration also occurs in this phase. The neovascularization and angiogenesis will be stimulated by capillary sprouting, following the movement of fibroblast along the fibrin network and re-epithelialization initiating from the wound edge. When apoptosis take place, the formation of granulation tissues stops. For all the necessary actions to occur, the chemical mediators and all the components of extracellular matrix will undergo numerous changes (Johnstone et al., 2005).

The physical endpoint of wound repair mechanism is the formation of a scar, which is related to the extent of the process of inflammation during wound healing (Jackson, Nesti and Tuan, 2012).

Types of wounds and wound healing

There are two major types in wound healing, depending on the type of wound. They are primary and

secondary wound healing. The below Figure 4 shows the differences between the two types of wound healing.

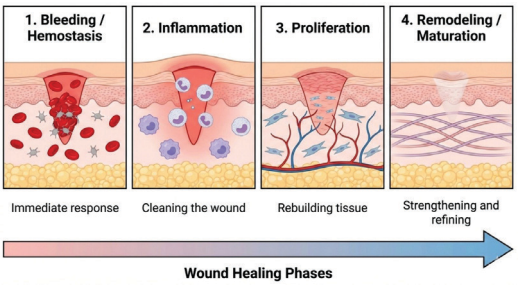

Figure 3: Phases of wound healing

Primary Healing	Secondary Healing
Wound is clean and uninfected.	There is extensive loss of cells and tissues
Edges of wound are approximated by surgical sutures	Wound is open with large tissue defect and at times infected
Takes place in surgically incised wounds	Edges of the wound are not approximated by surgical sutures.
Scar formation is neat and small	It forms the main bulk of secondary healing
There is no granulation tissue formation	Healing is slow
There is not much loss of cells and tissues	Healing takes place from base upwards besides from margins inward
Healing is rapid	

Figure 4: Comparison of primary and secondary wound healing.

Various types of traumas may cause various kinds of wounds. The classification can be made according to the cause of injury, severity of the wound and healing time .

Factors affecting wound healing

There are four major phases of wound. Numerous factors play a huge role in facilitating the wound healing process (Guo and Pietro, 2010). The factors can affect any of the pathway of the healing, therefore causing improper wound healing or even halt the process in between. Table 3 shows few local and systemic factors, which can affect any phase of wound healing.

Table 3: Factors affecting wound healing process.

Local factors	Systematic factors
Tissue hypoxia	Senescence
Contamination from incontinence	MaFlnourishment
Pressure	Smoking
Tissue endema	Stress
Necrotic material	Comorbidity
Infection	Immune copromise
Dessication	Obesity
Maceration	Diabetes, Anemia

Evolution of wound healing in the medical industry

The major goal of treating wounds is to prevent infection and removing redundant tissues from the body. There are many problems impair with wound healing and recovery of the injured site. It can even result in systemic pathology. Proper techniques of wound care not only prevent infection but also lead to quick recovery and even result in minimize scarring (Han and Ceilley, 2017).

In order to deliver proper treatment, the medical sector needs to work on several areas, including diagnostic, therapeutic, the research on therapeutic target for further drug discovery, prognosis and the prospects of health hazard. Various diseases related to wounds such as skin wound, corneal wounds, diabetes foot ulcers and chronic wounds are becoming major cause of disability or even death globally; numerous studies are ongoing on more effective treatments and therapeutics (Siddiqui and Bernstein, 2010). There are several techniques and methods that have been discovered, such as stem cells to treat wounds.

The progress of fields such as proteomics, genomics, bioinformatic, pathophysiology has led to an increasing interest in finding new therapeutic targets and exploring pre-existing targets (Zheng et al., 2006). This has a positive impact on modern drug discovery and novel methods and techniques in the medical sector. Hence, treating wounds is also improving with more effective novel treatment methods (Baltzis, Eleftheriadou and Veves, 2014).

Conclusion

The evidence present in this review has shown that successful treatment of wounds would be one of the major improvements in the medical field globally. As an initial step for therapeutic discovery, scientists have already found a therapeutic target of wound healing. Chemical mediators are one of the crucial factors for the future therapeutic and medical aspects. Which are normally involved in the immunological approach of the body towards inflammation arises from injuries and other diseases.

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3D Printed Antimicrobial Cups for Heavy Metal Chelation

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Introduction

Safe drinking water is a fundamental requirement for life. It also is a critical component for agriculture, irrigation, and commercial industries. Industrial water pollutants often include heavy metal ions such as lead, cadmium, copper, arsenic, and mercury. Exposed individuals to these suffer from numerous health issues including disorders in the renal, neurological, gastrointestinal, endocrine, immune, reproductive systems, and also skin diseases.

On the other hand, *Escherichia coli* (E. coli) is one of the bacterial species that are pathogenic to humans. Some of the *E. coli* serotypes, once present in water, lead to acute diarrheas and gastroenteritis. Hence, methods for the efficient removal of these types of contaminants from drinking water draw immense importance to the global community.

Most of the conventional water purification techniques (i.e. use of chemical agents like chelators, flocculants, organic dyes, and methods including filtration, reverse osmosis, and distillation) are optimized at industrial scale making them non-affordable for the general public. Moreover, when dilapidated infrastructure becomes the transportation mode of water, especially in areas of poor-living conditions, obtaining clean water becomes a major issue. With the target of addressing these challenges, we present a low-cost eco-friendly composite fabricated from chitosan and polylactic acid (PLA).

Chitosan contains lone electron pairs on the nitrogen atoms of the amine groups and oxygen atoms of the hydroxyl groups. These act as chelating sites for the heavy metal ions (Wu et al. 2001). On the other hand, electrostatic interactions between chitosan and negatively charged cell wall of *E. coli*, could disrupt the bacterial cell membrane, cause structural damage and leakage of cellular content inhibiting the bacterium. Our strategy in the present work was to combine chitosan with PLA, a biodegradable thermoplastic, forming a composite that could be 3D printed into free standing objects. After demonstrating toxic heavy metal chelation and antimicrobial properties for the composite material, cup-like robust structures could be 3D printed proving the potential capabilities to further enhance its performance via 3D printing, a growing technology that can achieve complex, high surface areas not conducive for conventional moulding (Appuhamillage et al. 2024).

Materials and Methods

PLA (Luminy LX175) in fine resin pellet form (melt flow index-MFI at 190 °C/2.16 kg) was received from Natur Tec Lanka (Pvt) Ltd, Sapugaskanda, Sri Lanka. Chitosan flakes (>= 75% deacetylated, molecular weight (Mw) 3,800-20,000 Da) was purchased from Sri SR Laboratory (Pvt) Ltd, Colombo 13, Sri Lanka. Lead (II) nitrate, Copper (II) nitrate trihydrate, and Cadmium (II) nitrate tetrahydrate were purchased in powder form from Athula Laboratory Equipment (Enterprises), Kaduwela, Sri Lanka. Ethylenediaminetetraacetic acid (EDTA) in powder form was purchased from Glorchem Enterprise, Colombo 11, Sri Lanka. Ultrapure water was obtained from a Nuve/NS 103 water purification system. Metal concentrations were analyzed using an Agilent 7900 inductively coupled plasma mass spectrometer (ICP-MS) under helium mode. All ICP-MS measurements were carried out using an aqueous solution containing 3% nitric acid and 2% hydrochloric acid as the matrix. Each measurement was calculated as an average of three measurements.

Preparation of composites

Neat PLA pellets and chitosan flakes were mechanically ground to 250 microns particle size. These powders were mechanically mixed homogeneously according to Table 1. Using a steel mould ((40 mm (length) × 40 mm (width) ×1 mm (thickness)), composites were prepared using a heat-press at 180 °C for 3 min under 0.3 MPa pressure.

Table 1. Composition of the composites in wt.%.

Material	PLA (wt%)	Chitosan (wt%)
Control (neat PLA)	100	0
10 C/PLA	90	10
20 C/PLA	80	20
30 C/PLA	70	30
40 C/PLA	60	40
50 C/PLA	50	50
60 C/PLA	40	60

Thermal characterization

As-prepared composites and neat PLA (the control) were subjected to TGA analysis using the TG analyzer (TGA 5500- Discovery TA) at 30-700 °C under a nitrogen atmosphere and at a 10 °C/min heating rate. DSC analysis was also performed using a DSC Q100-TA instrument in the 30-300 °C temperature range at a heating and cooling rate of 10 °C/min.

Heavy metal adsorption tests of the prepared composites

The as-prepared composite discs were completely and separately immersed in aqueous stock solutions of each metal ion in concentrations that represent moderately polluted water bodies (Das and Haldar 2017, Appuhamillage et al. 2019). For the detection of Pb^{2+} levels, a 30 ppb Pb^{2+} stock solution (250 mL) was prepared using the nitrate salt in ultra-pure water, and the immersed discs were subjected to mechanically stirring at 50 rpm at pH 7.0 and room temperature for 5, 10, 15, 30, and 60 min. After each time period, the supernatant was analyzed via ICP-MS. To detect Cu^{2+} and Cd^{2+} levels, the same procedure was carried out but using 1500 ppb and 30 ppb stock solutions prepared using the corresponding metal nitrate salt respectively. Neat PLA was used as the control at each occasion.

Antimicrobial activity

As a proof of the concept, the antimicrobial activity of the composites 30 C/PLA and 60 C/PLA was investigated against Gram-positive strains such as *Staphylococcus aureus* (ATCC 6538) and *Bacillus cereus* (ATCC 14579) and Gram-negative *Escherichia coli* (ATCC 8099). The agar diffusion method was followed (Zhang et al. 2015) with minor adjustments.

3D Printing

Fused filament fabrication (FFF) based 3D printability was evaluated for the prepared composites, starting from the lowest chitosan loaded 10 C/PLA material. Using the 10 C/PLA, 20 C/PLA and 30 C/PLA composites, 3D printable filaments having a square-shaped cross- section (dimension: 1.24 mm (W) ×1.24 mm (H) ×20 cm (L)) were prepared with a stainless steel mould of same dimensions, under the heat-press conditions mentioned before. Using these filaments, cup-like shapes of 20 mm outer diameter, 0.4 mm wall thickness, and 10 mm height were 3D printed via a FFF 3D printer (Creality-Ender 3). The 30 C/PLA was also 3D printed into a complex object with pass-through holes and estimated total surface area of ca 2,413 mm^2.

Mechanical properties of 3D printed cups

A universal testing machine (Testometric-M500-50CT Win-Test) was used for the compression tests that were performed on the 3D printed 30 C/PLA cups. A compression rate of 5 mm/min was used at room temperature conditions. Ultimate compressive strength, toughness, and elastic Young's modulus were determined as averages from three measurements. PLA was used as the control.

Results and Discussion

Heavy metal adsorption tests of the prepared composites

As per the results shown in Figure 1, 30 C/PLA and 60 C/PLA composites were capable of producing safe drinking water within 5 min of contact time with Pb^{2+} solution, as the remaining Pb^{2+} concentration goes below the EPA level of 15 ppb (denoted by the dotted line in Figure 1) within 5 min. Further, all the three composites show significantly higher Pb^{2+} adsorption than that of neat PLA, the control, within all the contact times tested.

Antimicrobial activity

As per the results illustrated in Figure 2, inhibition zones were observed for the Gram-negative pathogenic

strain *E. coli* (ATCC 8099) for the 30 C/PLA and 60 C/PLA composites. In fact, the circular film diameter with the inhibition zone resulted for 60 C/PLA was slightly higher (13.5 mm) than that of the 30 C/PLA (12.0 mm). No inhibition zone was observed for neat PLA, the control.

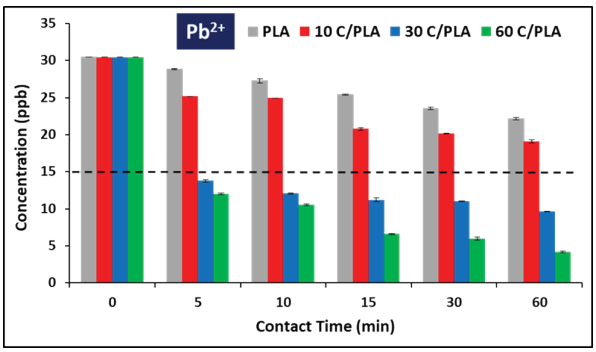
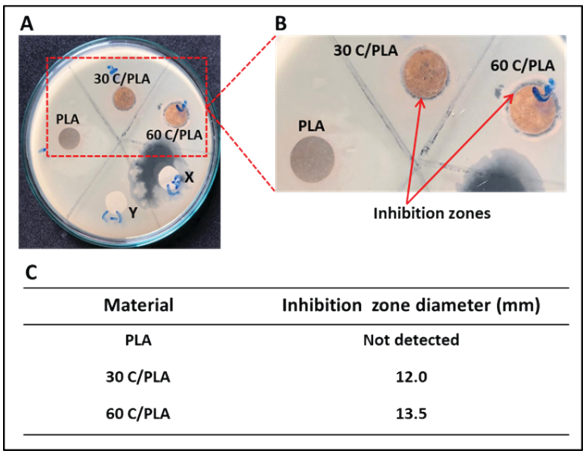


Figure 1: Comparison of the remaining Pb2+ concentrations in solution for 10 C/PLA, 30 C/PLA, 60 C/PLA, and neat PLA. EPA action level (15 ppb for Pb2+) is shown in black dotted line. A contact time of 0 min represents the initial Pb2+ concentration (30 ppb) in the stock solution. Adapted from Wijenayake et al. 2025.



C

Material	Inhibition zone diameter (mm)
PLA	Not detected
30 C/PLA	12.0
60 C/PLA	13.5

Figure 2: Antimicrobial activity tests. (A) Agar plate containing the circular film discs of neat PLA, 30 C/PLA, 60 C/PLA composites, the positive- control Amoxicillin (labeled X), and blank filter paper disc as the negative-control (labeled Y). (B) Zoomed section of the agar plate showing the inhibition zones of 30 C/PLA and 60 C/PLA against E. coli (ATCC 8099), and (C) resulting inhibition zone diameter (mm) vs. material used against E. coli (ATCC 8099). Adapted from Wijenayake et al. 2025.

3D Printing

In order to test whether we could use the C/PLA composite to fabricate a free-standing object that could be practically applied as a water filtration device, FFF- based 3D printing was carried out starting from the lowest chitosan loaded 10 C/PLA composite. According to the results depicted in Figure 3 (A), cup-like shapes could be successfully 3D printed using the composites; 10 C/PLA, 20 C/PLA, 30 C/PLA, and neat PLA. Furthermore, the 30 C/PLA material was also successfully 3D printed into a more complex free-standing object having pass-through holes and an estimated total surface area of ca 2,413 mm^2, as shown in Figure 3 (D). This proved that the chitosan/PLA composite, as a toxic heavy metal adsorbent, has the potential to be further developed into more complex geometries with internal cavities and high surface areas via 3D printing, which is not conducive easily by conventional moulding techniques like injection moulding.

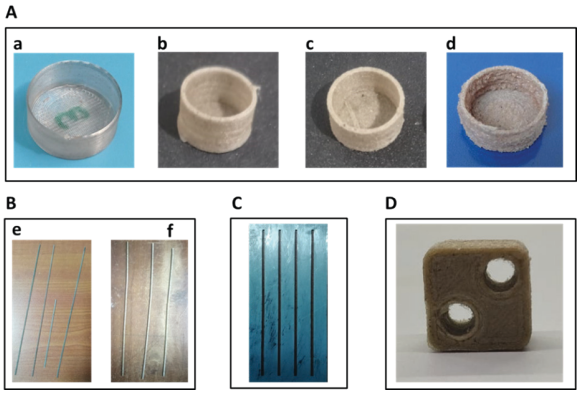


Figure 3: 3D printing of composites. (A) 3D printed cup-like shapes using neat PLA (a), 10 C/PLA (b), 20 C/PLA (c), and 30 C/PLA (d). (B) Representative filaments prepared for 3D printing using neat PLA (e) and 30 C/PLA (f). (C) A set of four steel moulds (dimension of one: 1.24 mm (W) ×1.24 mm (H) ×20 cm (L)) used to prepare the filaments. (D) 3D printed free-standing complex geometry with an estimated total surface area of ca 2,413 mm^2 using 30 C/PLA. Adapted from Wijenayake et al. 2025.

Mechanical properties of 3D printed cups

As per the results shown in Figure 4, all the mechanical properties; ultimate compressive strength, toughness, and Young's elastic modulus had been

significantly improved in the 30 C/PLA composite compared with neat PLA, the control.

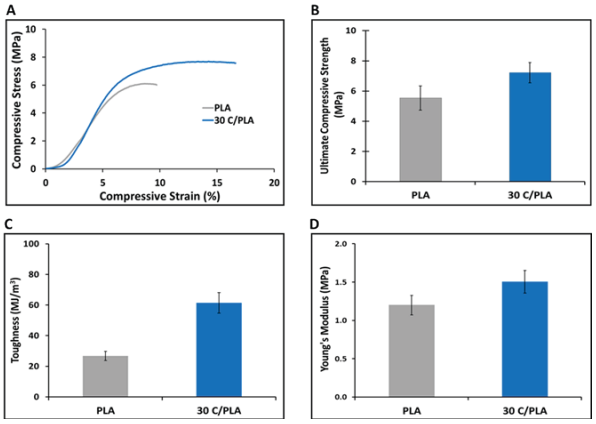


Figure 4: Resulting mechanical properties of the 3D printed 30 C/PLA cups against neat PLA. (A) Representative stress vs. strain plots of 3D printed neat PLA and 30 C/PLA cups. (B), (C), and (D) depict the comparison of ultimate compressive strength, toughness, and Young's modulus of the 3D printed 30 C/PLA cups vs. neat PLA, respectively. Adapted from Wijenayake et al. 2025.

Conclusions and future work

In conclusion, the work reported here introduced a direct fabrication of eco-friendly 3D printable antimicrobial composite that has the ability to capture toxic heavy metal ions from contaminated water. For the first time, a 3D printable biodegradable chitosan/PLA composite (30 C/PLA) has reduced toxic Pb^{2+} levels below EPA-AL before 5 min and shown reusability achieving ca 96% of the original Pb^{2+} adsorption efficiency even after the fifth regeneration cycle. This material has also shown antimicrobial properties against *Escherichia coli*, a bacterium that could live in water. The additively manufactured cups of 30 C/PLA resulted significantly improved compressive strength, toughness, and Young's modulus with respect to neat PLA, the control.

Moreover, a separate study would evaluate the effects of other parameters such as pH of the medium, concentration of competing/coexisting ions, and temperature on the metal adsorption kinetics of the composites. The effect of adsorbent surface area on metal filtration efficiency would also be evaluated by fabricating 3D printed geometries with high surface areas and directly applying for heavy metal adsorption in water.

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Advancing Sri Lankan Research: The Emerging Role of Computational Science

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Introduction

In modern scientific research, computation has risen to the forefront as a powerful driver of discovery, alongside theory and experiment. Nowadays, computational research ranges from modeling protein dynamics and predicting climate patterns to analyzing large scale social data and optimizing engineering designs. While many countries have identified computational research as a key contributor to national development and invested heavily in computational infrastructure, others are still in the process of fully integrating computational research into their scientific and development strategies. For a country like Sri Lanka, rich in intellectual talent but constrained by limited resources, computational research is not merely an option; it is a strategic opportunity. Popularizing computational research among Sri Lankan researchers can accelerate innovation and open the access to high impact science. This article explores why computational research matters for Sri Lanka, the barriers that limit its widespread adoption, and the practical steps needed to start a strong, sustainable computational research culture in the country.

Why Computational Research Matters for Sri Lanka?

Traditional experimental research typically depends on costly laboratory infrastructure, including highly specialized instruments, recurring consumables, and continuous maintenance. In contrast, computational research primarily relies on advanced algorithms and access to reliable yet increasingly affordable computing resources (Figure 1), making it a more cost-effective and scalable approach for many scientific investigations. Therefore, computational research substantially lowers the entry barrier for scientists to internationally competitive research, particularly in institutions where funding is unavailable or extremely limited.

Figure 1: Affordable workstations in the Computational Biophysics Laboratory, Department of Chemistry, University of Sri Jayewardenepura.

Globally, funding agencies, journals, and industry increasingly value computational research approaches in many fields. Hybrid studies that integrate simulation, modeling, and data analytics with experiments are frequently appearing in the high impact journals like Nature and Science. Positively managing this trend, Sri Lankan researchers with strong computational skills can position themselves on the global stage more effectively by publishing in high impact journals and competing for global research funding.

One of the greatest advantages of computational research is the availability of powerful open source software. Sri Lankan researchers can benefit immensely from tools such as ORCA and GAMESS for quantum chemical calculations, GROMACS, LAMMPS, and NAMD for molecular simulations, R, Python and Octave for statistics and data analysis, rather than relying on expensive commercial products.

Sri Lanka has an excellent pool of researchers in universities and research institutes, many of whom possess strong experimental and theoretical backgrounds in physics, chemistry, biology and mathematics. Despite notable progress by individual researchers and small groups in modeling, data analytics,

and simulation-based research using open-source tools and international collaborations, computational research remains far from widely adopted in Sri Lanka.

Barriers to Popularization

The growth of computational research in Sri Lanka is restricted by several barriers. One of the main barriers is funding constraints. Many Sri Lankan research grants place strict caps on equipment budgets, often treating computational hardware as a secondary or non essential expense. As a result, researchers are forced to rely on entry level systems that significantly slow simulations and data analysis. Moreover, inadequate funding limits the training of local workforce in computational research. While Sri Lankan students excel in theory, structured training in scientific computing is often missing from undergraduate and postgraduate curricula. Without systematic training, advanced methods such as molecular dynamics, finite element modeling, or machine learning remain inaccessible. Another major challenge for computational research is that researchers in this field often work in isolation, with few opportunities for peer learning, knowledge sharing, and meaningful collaboration within the country. The absence of strong national networks or forums reduces knowledge sharing and slows collective progress. The decision-making body of many Sri Lankan institutes has a persistent misconception that computational research is merely supportive of experimental work. This perception undervalues in silico experiments that can generate independent hypotheses testing. In evaluation processes, such as thesis assessments, promotions, and grant reviews, computational work is usually scrutinized improperly by non specialist panels.

Strategies to Popularize Computational Research

To popularize computational research among Sri Lankan researchers, exposure must begin early. Universities should introduce compulsory courses in scientific programming (Python, R, MATLAB, C++) and embed these components into core science subjects. Postgraduate programs should recognize computational theses as standalone research contributions, not merely supplements to experiments. Sri Lanka needs to substantially improve access to computing resources, which at present remains severely limited. Funding agencies and research councils can play a pivotal role by recognizing computational hardware as a core research infrastructure and allocating enough funding to acquire enough computational power. If distributing limited funds across many computational proposals is challenging, institutions can develop shared departmental or inter university computing clusters. Government can contribute to the development of computational research by establishing national level supercomputing centers. Although the initial investment required for such an initiative is substantial, the benefits will be long-term and sustainable. In addition to the points above, international collaborations can immediately provide local researchers with access to advanced facilities that are currently unavailable in Sri Lanka, though the approach is not sustainable.

Conclusion

The future of Sri Lankan research does not lie solely in building more laboratories, but in empowering minds with the tools to model, simulate, and analyze the world digitally. By adopting computational research through education, infrastructure, policy reform, and community building, Sri Lanka can unlock a new era of scientific productivity and global engagement. Popularizing computational research is, ultimately, about believing that world class research can be done anywhere, provided curiosity is matched with capability. In that belief lies Sri Lanka's greatest research opportunity.

55th Annual Sessions of the Institute of Chemistry Ceylon 2026

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  For research predominately in basic Chemistry (Organic, Inorganic, Physical, and Analytical).

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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 thecontent.

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  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.

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  Awarded for the best research paper presented at the Annual Sessions of the Institute of Chemistry Ceylon, for work carried out and completed in Sri Lanka.

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