**A look at the improvement of the scientific system in the seventh development plan of the country**

Ali Akbar Saboury

**Abstract**

The 20th chapter of Iran’s seventh Development Plan (2024-2028), titled "Upgrading the Scientific, Technological, and Research System," outlines ambitious goals for the country’s scientific advancement. Iran aims to achieve a global ranking of 14 in science production, rank 50 in inventions, and reach 42nd place in the Global Innovation Index (GII). However, these targets appear unrealistic given Iran’s declining rankings in recent years. The plan also aims to double the annual per capita number of internationally indexed articles to 1.5, which seems unattainable under current conditions. Additionally, while the country aspires to have 20 universities ranked below 500 and attract 320,000 foreign students, the ranking of Iran’s top universities has worsened in recent years. Iran has a strong foundation in developing skilled human resources, but poor planning has led to significant brain drain. Achieving these goals requires a clear understanding of the current scientific landscape, substantial investment in research infrastructure, and effective science policy-making. The 7th plan, as it stands, appears overly optimistic and disconnected from the realities of Iran’s scientific and educational challenges.

**Keywords:** Scientometry, Seventh development plan, University rank, Global Innovation Index (GII), Invention rank

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**Current status and challenges of herbal-derived exosome-like nanoparticles in pharmacy**

**Current status and challenges of herbal-derived exosome-like nanoparticles in pharmacy**

Atefeh Alipour

**Abstract**

Due to the complex etiology of various diseases like cancers and the side effects of conventional drugs, researchers have concentrated on finding novel treatments approaches with higher efficiency and safety. Moreover, current delivery systems for therapeutic drugs such as synthetic nanoparticles can cause serious DNA or RNA damage, inflammation, improper immune reactivity, and other side effects. Natural exosomes majorly herbal-derived exosomes have been found to be capable of efficient loading chemical or nucleic acid drugs to target tissues with great potential for several applications. Here, we summarize the prospect of plant exosome targeting delivery systems with less challenges compare to mammalian-derived exosomes to transport multiple molecules to target cells even affecting intestinal transporters and discuss about their biochemical characteristics, inherent biological functions as well as their effectual production in large quantities with lower costs. Further, necessity of further research required for the selection of suitable herbal sources and purification approaches for their feasible mass production and plan for extending their future applications in pharmacy and cosmeceutical will be debated.

***Keywords:*** Plant-derived exosomes, Target Drug delivery, Prospective pharmacy, Cancer

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**Biophysical and biochemical approaches to direct stem cells trans-differentiation for bone repair**

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**Abstract**

Biophysical and biochemical cues are critical factors in designing an artificial niche for tissue repair and regeneration in clinical application due to their vital role on controlling stem cell differentiational abilities. Specifically, identification of crucial biophysical and biochemical cues of biomaterials that can synergistically recapitulate the osteoblast microenvironment will be of particular importance for proper bone regeneration. Present study aims to provide a comprehensive and systematic understanding mechanistic detail of several qualities of matrix properties such as geometry, topography, capability of delivering growth factors, inducers, small bioactive molecules, and genetic regulators that influence stem cell attachment, proliferation, and differentiation for promoting osteogenesis. We highlight recent advances on various microenvironmental indications such as mechanical forces within, and viscoelastic properties and chemical competence of osteo inductive materials able to solve reproducibility, scalability, incurred cost, and biocompatibility challenges and discuss how they can be improved for precise bone tissue engineering. Integrating of biophysical and biochemical cues would potentially shed the light to make next-generation functional biomaterials for diverse applications in regenerative medicine in the near future.

***Keywords:*** Bone regeneration, Cell niche, Stem cell therapy, Viscoelastic properties, Scaffolds

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**The effects of unfolded protein response inducing agents in cell apoptosis**

Reyhaneh Golezaria, Sanaz Nour-Mohammadzadehb, Ali Abedib, Mojtaba Amania,c

**Abstract**

Proteins are vital macromolecules that perform essential cellular functions. They achieve their specific three-dimensional structures through folding. Misfolded or unfolded proteins can lead to proteotoxic stress, cellular dysfunction, and tissue damage, contributing to chronic diseases like Alzheimer’s, Parkinson’s, Huntington’s, and various cancers. Cells employ several mechanisms to ensure proper protein folding, including chaperones, the ubiquitin-proteasome system, co-translational control, and quality control networks such as the integrated stress response (ISR) and unfolded protein response (UPR). The UPR is crucial for cancer cell survival, as it helps restore protein homeostasis by reducing transcription, enhancing folding capacity, and degrading misfolded proteins. Intrinsic and extrinsic stresses—such as hypoxia, glucose depletion, lactic acidosis, oxidative stress, low pH, and errors in glycoprotein and lipid biosynthesis—heighten the demands for protein translation and secretion in malignancies, further stressing the protein secretory pathway and increasing misfolded protein levels. Depending on the duration and severity of proteotoxic stress, the UPR can activate survival signals through adaptive and anti-apoptotic pathways or induce cell death programs. Therefore, pharmacologically inducing pro-apoptotic UPR or inhibiting pro-survival UPR may offer therapeutic benefits in cancer treatment. This study investigates the effects of chronic UPR induction by combining 2DG and Metformin—two drugs that induce UPR through different mechanisms—on the AML-related KG1a cell line. Results indicate that these drugs induce cell death by upregulating pro-apoptotic UPR genes, including ATF4, ATF5, and CHOP. Additionally, another study found a direct correlation between elevated levels of UPR markers ATF4 and ATF6 and the stage and grade of endometrial cancer, suggesting their significant role in cancer progression and prognosis.

***Keywords****:* Proteins, Biosynthesis, Stem cell therapy, Viscoelastic properties, Scaffolds

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**Development of novel peptide ligands for enhanced drug delivery and tumor imaging**

S. Mohsen Asghari

**Abstract**

In preclinical precision oncology, enhancing tumor imaging is crucial for early cancer detection, accurate diagnosis, and effective monitoring of treatment responses. Nanotechnology and molecular imaging advancements have enabled the development of novel imaging agents with remarkable sensitivity and specificity. This presentation explores innovative strategies using tumor-targeting peptides, focusing on the dual-targeting peptide VGB3, which binds to vascular endothelial growth factor receptors 1 (VEGFR1) and 2 (VEGFR2), and the endostatin-derived peptide C-peptide to improve tumor imaging across various modalities. VEGFR1, VEGFR2, and integrins, highly expressed in tumor cells and the tumor microenvironment, serve as effective imaging targets.

Our research investigates conjugating these peptides with imaging agents to enhance targeting efficacy. We developed VGB3-DOTA-Gd and VGB3-DTPA-68Ga conjugates, which significantly improve PET and MRI imaging for precise tumor localization. Incorporation of C-peptide into solid lipid nanoparticles (SLNs) enhances delivery, stability, and biocompatibility of imaging agents. Furthermore, superparamagnetic iron oxide nanoparticles (SPIONs) conjugated with C-peptide provide high-contrast MRI imaging of tumor tissues. Gold nanoparticles decorated with C-peptide have been synthesized to enable dual-modality imaging for CT and MRI, achieving comprehensive tumor visualization.

This presentation offers an in-depth overview of our laboratory’s pioneering strategies for employing tumor-targeting peptides to advance imaging techniques. Our findings underscore the importance of integrating targeted peptides with advanced imaging agents for improved cancer diagnostics, paving the way for enhanced patient outcomes in oncology.

***Keywords:*** Tumor targeting, Peptides, Magnetic resonance imaging, Positron emission tomography, Computed tomography

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**Split reporter-protein complementation strategy for detecting regulated proteins interaction in apoptosis signaling**

FarangisAtaei

**Abstract**

Inhibitor of apoptosis (IAP) protein represents a group of negative regulators of caspases and cell death signaling. XIAP is a direct inhibitor of cell-death proteases, caspase-3/7, and -9. SMAC regulates XIAP function and potentiates caspase-3/7 and -9 activity by disrupting the interaction of caspases with XIAP. The binding of SMAC to the BIR2 and BIR3 regions of XIAP creates a steric hindrance that is essential for preventing binding of XIAP with caspases, thus achieving neutralization of XIAP inhibition and promoting the release of XIAP from caspase-9-apoptosome complex. Here, we used split luciferase (Luc) complementation assay for the exploration of protein-protein interaction. The non-functional fragments, NLuc and CLuc, were used to create fusion models which can be assembled into a functional protein by interacting the fused proteins of interest. Based on this strategy, fusion models of caspase-3, caspase-9, some truncated XIAP with BIR2 and/or BIR3, and mature SMAC were expressed in bacterial host and purified. To effectively detect conformational rearrangement resulting from interaction, the pairwise samples were mixed together and measured the signal produced. After various optimization under different cognitions, our finding indicates that the length of truncated proteins, linker and condition media are the important parameters in the design of fusion proteins, especially in spilt-complementation method. Taken together, an in vitro bioluminescence assay for direct measurement of IAP interaction with caspase-3, -9 and SMAC was successfully created that can be used to monitor various compounds that target these interactions to provide predictive insights.

***Keywords:*** Split-luciferase, XIAP, Caspase 3, Caspase 9, SMAC, Interaction assay

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**Bioinformatic analysis of expression data in multiple sclerosis**

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**Abstract**

Multiple sclerosis (MS) is an autoimmune neurodegenerative disease whose prevalence has increased. MS is a disease that destroys the myelin sheath of nerve cells in the central nervous system. In the present study, microarray technology and bioinformatics tools were used to identify genes and their interaction pathways to investigate common molecular mechanisms. Additionally, on the basis of the results of this analysis, drug predictions for the treatment of MS were made. Microarray data from the NCBI database, specifically from the gene expression omnibus (GEO) section related to GSE41890, containing information on gene expression in 68 samples, were extracted. The two groups, normal and treatment, were subsequently compared. The R programming language was used to analyze the differentially expressed genes (DEGs), and the desired molecular network was constructed. The protein‒protein interaction (PPI) network was created via STRING, and PPI network module analysis was performed via Cytoscape. To investigate protein‒drug interactions, NetworkAnalyst was used. Finally, docking operations were performed via PyRx software. A total of 1190 DEGs, which were involved mainly in cell immunity, the cell cycle, cell proliferation, and signal transduction, were identified. The PPI network contained 67 nodes and 629 interactions. Three protein targets and fifty-one drug candidates were identified; specifically, approximately 11 drugs were linked to KIF11, 33 drugs were linked to CCNA2, and 7 drugs were linked to CDK1. A total of 99443535, 5005498, and 4566 compounds were generally connected to KIF11, CDK1, and CCNA2, respectively.

***Keywords:*** Multiple sclerosis, Microarray, Gene, Protein-protein interaction, Docking

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**Assessment of fish skin grafts in the burn wound healing through synchrotron FT-IR micro spectroscopy**

Maryam Mitra Elmia, Fatemeh Elmib,\*, Armita Hodac

**Abstract**

The application of fish skin grafts in the management of burn injuries has garnered significant interest recently due to their distinctive properties. This research focuses on the healing process of wounds in a rat model following third-degree burns. During the healing phase, the rat skin exhibits various structural and molecular alterations, particularly concerning proteins and lipids. In this study, synchrotron radiation Fourier-transform infrared micro spectroscopy (SR-FTIRM) was employed to examine the dermal region of rat skin post third-degree burns. The experiment involved three groups of rats: one group received treatment with white fish skin, another with carpio fish skin, and a control group with untreated wounds. The analysis of collagen fiber orientation, determined by the ratio of amide I to amide II (integrated intensities: 1600-1710 cm-1/1492-1598 cm-1), revealed that the group treated with white fish skin exhibited the most organized arrangement of fibers. Gaining insights into such structural characteristics may significantly improve our comprehension of wound healing mechanisms and tissue regeneration.

***Keywords:*** Fish skin graft, Burned wound healing, Collagen, Synchrotron radiation FT-IR micro spectroscopy

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**The conformational transition of prion to β-strands in prion fibrillation from molecular dynamics simulations**

Sattar Khashkhashi-Moghadama,†, Anahita Khammarib,c,†, Seyed Shahriar Arabb,\*, Ali Akbar Sabouryc,\*

**Abstract**

Prion diseases, such as Creutzfeldt–Jakob disease, Gerstmann- Straussler- Scheinker syndrome, and fatal familial insomnia, are caused by the conversion of the cellular prion protein (PrPC) into an insoluble, beta-sheet-rich, infectious isoform (PrPSc). Structurally, this transformation involves the transition of the second and third α-helices in the prion C-terminal region into β-strands, which are stabilized by a disulfide bond in prion fibrils. Through targeted molecular dynamics simulations, we identified critical regions in the prion sequence that initiate fibril formation under physiological conditions. Notably, regions 172-176, 190-200, and 220-224 showed early deformation and loss of structure during simulations. We also realized the prion C-terminal mutations disrupt hydrophobic interactions, destabilize electrostatic interactions and salt bridges, cause side-chain interference, or damage the hydrogen bond networks that enhance structural instability and promote amyloid fibril formation. This study provides molecular insights into the early stages of the prion fibrillation mechanism.

***Keywords:*** α-β structural transition, Prion fibril formation, Aggregation-prone sites, Targeted molecular dynamics simulation

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**Investigating the Antimicrobial and Anti-biofilm Effective of Active Plant Compounds on Streptococcus mutans: A Bioinformatics Study**

Zahra Zahmatkesh Saraidashti\*, Mansoreh Hosseini, Nasim Babak Nezhad, Sanaz Behnam

**Abstract**

Dental caries is one of the most common and costly biofilm-related infectious diseases worldwide. Streptococcus mutans has been identified as the main cause of caries due to its synthesis of extracellular polymeric substances and the creation of acidic conditions. Increasing resistance of microorganisms to antibiotics has become a scientific concern. Increasing resistance of microorganisms to antibiotics has become a scientific concern. The increasing resistance of microorganisms to antibiotics has become a scientific hazard. To date, many secondary plant compounds have been identified with diverse biological activities including antibacterial, antifungal and anticancer activities. Therefore, in this study, screening plant antimicrobial agents affected and affected these compounds. First, natural plant compounds were retrieved from the database. After optimizing the structure and investigating ligand-protein interactions, the desired plant compounds were examined for physicochemical properties. In this study, all plant compounds were included in the three main groups of flavonoids, terpenoids and alkaloids using virtual screening. The database was also searched using keywords and their combinations. For the purpose of herbal compounds, the base and given compounds with confirmed anti-alveolitis activities were investigated. According to the results, the secondary herbal compounds have a bond with glucosyltransferase enzymes. Therefore, they were used as natural materials for natural antibacterial compounds and to prevent oral plaque and biofilm formation by S. mutans.

***Keywords:*** Tooth decay, Streptococcus mutans, Plant secondary compounds, Glucosyltransferase, Flavonoids, Terpenoids and alkaloids

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**The potential of cell-penetrating peptides in neurodegenerative disease management and drug delivery**

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**Abstract**

Cell-penetrating peptides (CPPs), also referred to as Trojan peptides or protein translocation domains, have emerged as a highly promising platform for intracellular delivery of polar and hydrophilic therapeutic agents, including peptides, proteins, and oligonucleotides. These peptides offer a noninvasive, efficient solution to the limitations associated with conventional delivery methods, such as low efficacy, high toxicity, and poor bioavailability. CPPs can traverse biological membranes to facilitate the transport of therapeutic molecules into challenging tissues, notably the central nervous system, by crossing the blood-brain barrier. This capability positions CPPs as valuable candidates for treating neurodegenerative diseases such as Alzheimer’s and Parkinson’s disease. Moreover, CPPs exhibit potential in mitigating pathological protein aggregation, a common feature of neurodegenerative conditions characterized by amyloid formation. Recent findings from our group demonstrate that the CPP-derived peptide p216 effectively targets and neutralizes toxic α-synuclein oligomers associated with Parkinson’s disease, thereby reducing oligomer-induced cytotoxicity. These results highlight the versatility of CPPs as a robust tool for advancing both basic research and therapeutic strategies in the treatment of neurodegenerative disorders.

***Keywords:*** Cell-penetrating peptides, Blood-brain barrier, Neurodegenerative disease, Protein aggregation

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**The effects of two fractions isolated from scorpion venom in inhibiting proliferation and inducing apoptosis of HepG2 cancer cell line**

Zahra Setayesh-Mehr

**Abstract**

In the present study, the activity of two fractions of Hemiscorpius lepturus venom was investigated in vitro. In the first step, the effects of cytotoxicity fractions 2 and 4 (F2 and F4) purified from scorpion venom were measured. Thus, the cells were treated with different concentrations of F2 and F4 (0-50 µg/ml) for 24 hours. In the second step, the process of cell death was evaluated through the Real Time PCR technique to check the expression level of the genes involved in the apoptosis process. In the gene expression measurement phase, cancer cells were treated with two concentrations of F2 and F4 for 24 hours. The results of the present study showed that increasing the concentration of the purified fractions is associated with a significant decrease in the percentage of cell viability (p<0.05) and it was reported that F2 at a concentration of 20.41 µg/ml and F4 at a concentration of 20/µg/ml 37.54 ml caused the death of 50% of the cells. The results related to gene expression showed that increasing the concentration of both fractions was associated with a significant increase in the expression of Bax and cytochrome c genes, while the expression of Bcl-2 gene was decreased (p<0.05). In general, it seems that the cytotoxic effect of two fractions obtained from scorpion venom is related to their apoptosis induction effect through the mitochondrial pathway. Therefore, H. lepturus scorpion venom may be an interesting natural extract for further research in liver cancer treatment strategies.

***Keywords:*** Scorpion venom, *Hemiscorpius lepturus*, Viability, Apoptosis, Gene expression

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**Antiproliferative effect of Iranian scorpion Hemiscorpius lepturus venom in vitro on Caco2 cancer cell line**

Zahra Setayesh-Mehr

**Abstract**

The venom of some species of scorpions causes apoptosis and stops the proliferation of cancer cells. This important feature can be used in the isolation of therapeutically important compounds in cancer research. In the present study, the cytotoxicity effects of two fractions 2 and 4 (F2 and F4) separated by HPLC from *Hemiscorpius lepturus* venom were evaluated *in- vitro*. First, cytotoxicity was evaluated using MTT assay. After cultivating Caco2 cells in MTT test, different concentrations of F2 and F4 (0-180 µg/ml) were added to each well and treated for 24 hours. Then the process of cell apoptosis was investigated by measuring the expression of Bax genes, caspases 3 and 9 by Real Time PCR technique. The results showed that by increasing the concentration of both fractions, the survival percentage of cancer cells treated with F2 and F4 decreased significantly compared to untreated cancer cells (p<0.05). The IC50 values ​​for F2 and F4 were 80.24 µg/ml and 74.64 µg/ml, respectively. The results of gene expression showed that the expression of Bax, caspase 3 and 9 genes in cancer cells treated with two fractions increased significantly compared to untreated cancer cells (p<0.05). Finally, the increased expression of caspase and Bax genes after treatment with both purified fractions of scorpion venom confirmed the apoptotic properties of F2 and F4. These results show that *H. lepturus* scorpion venom can be a potential source for isolating effective molecules in the process of anti-proliferation and apoptosis of cancer cells.

***Keywords:*** Scorpion venom, *Hemiscorpius lepturus*, MTT, Apoptosis, Gene expression

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**Biophysical impacts of ionic strength and salt type on gelation of soy protein isolate**

Soroush Behjati Hosseini\*, Payam Arghavani, A.A. Moosavi Movahedi

**Abstract**

This study investigates the impact of salt capacity on Soy Protein Isolate (SPI) gelation, a crucial process in food and biomaterial development. The significance of metal salts as powerful crosslinkers to form hydrogels is of interest in biomaterial science. We found that SPI gelation relies on protein denaturation and aggregation into a three-dimensional network, influenced by pH, temperature, and ionic strength. It was indicated that chloride salts can improve SPI gelation potential. The research examined the role of Li+, Na+, K+, Ca2+, Mg2+, Mn2+, Fe3+, and Al3+ cations in SPI gel formation using three SPI concentrations (10, 15, and 20 mg/mL) at pH 2.0, heated at 85°C for varying times. Factors affecting gel formation were analyzed both separately and simultaneously, with a visual assessment conducted to determine gel formation. The results indicated that a minimum SPI concentration of 15 mg/mL is necessary for gel formation, with a minimum processing time of 4 hours. For monovalent cations, no gel formation at 50 mM occurred. In contrast, both monovalent and divalent salts enabled gel formation at concentrations of 100 and 150 mM. The gelation capability of Mg2+ and Mn2+ was more pronounced. Notably, none of the trivalent cations led to SPI gelation. These findings underscore the significance of salt type and concentration in modulating SPI gelation, providing valuable insights for applications in food and biomaterial science.

***Keywords:*** Soy protein isolate, Gel formation, Metal salts, Crosslinker

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**Antioxidant activity of *Hemiscorpius lepturus* venom fractions: Evaluation of radical scavenging potential**

Zahra Setayesh-Mehr

**Abstract**

Given the lack of side effects, antioxidants extracted from natural sources have attracted considerable attention from researchers. The present study aimed to evaluate the activity of two fractions, F2 and F4, isolated from *Hemiscorpius lepturus* venom. For this purpose, the two isolated were evaluated for their antioxidant activity using various assays, including 1,1-diphenyl-2-picrylhydrazyl (DPPH), 2,2-azino-bis (3-ethylbenzothiazoline-6-sulfonic acid) (ABTS+), and hydroxyl free radicals. The results showed that as the concentration increased, both fractions demonstrated enhanced radical scavenging ability. Additionally, there was no significant difference in the radical scavenging effectiveness between the two fractions and the positive control. The IC50 values ​​for the two fractions were as follows: for DPPH radical scavenging, 17.49 µg/mL for F2 and 15.10 µg/mL for F4; for ABTS radical scavenging, 20.90 µg/mL for F2 and 20.43 µg/mL for F4; and for hydroxyl radical scavenging, 26.69 µg/mL for F2 and 25.75 µg/mL for F4. In general, the results of the present study showed that the two isolated fractions, F2 and F4, could be promising new antioxidant agents warranting further investigations.

*Keywords:* Fraction, Scorpion venom, *Hemiscorpius lepturus*, Antioxidant, *In- vitro*

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**Investigating fractions extracted from scorpion venom on catalase enzyme activity in HEK293 human embryonic kidney cells**

Zahra Setayesh-Mehr

**Abstract**

In this study, the effect of fractions extracted from Hemiscorpius lepturus scorpion venom on HEK293 human embryonic kidney cells was investigated in the presence and absence of H2O2. The survival percentage of cultured cells was measured using MTT test. For this purpose, different concentrations of two fractions F2 and F4 (0-35 µg/ml) were prepared. In addition, catalase enzyme was extracted from the cells and then its activity was measured. The results of the study showed that the survival percentage of HEK293 cells treated with F2 and F4 decreased in the presence and absence of H2O2 depending on the dose. The decrease in survival percentage at the concentration of 35 µg/ml, for both fractions F2 and F4, was 22.45% in the absence of H2O2 and 18.5% in the presence of H2O2 compared to the untreated control sample. Both F2 and F4 fractions neutralized the reduction of catalase enzyme activity, so they were able to increase the activity of catalase enzyme in the presence of H2O2 compared to the absence of H2O2. The increase in catalase activity for cells treated with F2 and F4 was, respectively, in the absence of H2O2 (28 and 61%) and in the presence of H2O2 (47 and 63%). In general, the results of the present study showed that F2 and F4 extracted from scorpion venom, through their antioxidant activity, increase the survival rate and also increase the activity of catalase enzyme.

***Keywords:*** Fraction, Scorpion venom, *Hemiscorpius lepturus*, HEK293, Antioxidant

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**UiO66-NH2** **coated polyaniline nanocomposite for the adsorption of antiradical biomolecule quercetin: A kinetic and thermodynamic insight**

Azam Jabbari\*, Morteza Jabbari, Ehsan Nazarzadeh Zare

**Abstract**

In this study, UIO66-NH2 coated polyaniline (UIO66-NH2@PANI) nanocomposite was synthesized using a straightforward step-by-step self-assembly method and evaluated for selective adsorption of the antiradical biomolecule quercetin. The synthesized UIO66-NH2@PANI nanocomposite underwent comprehensive structural and thermal characterization using Fourier-transform infrared spectroscopy (FT-IR) and thermogravimetric analysis (TGA). The adsorption behavior of quercetin onto the nanocomposite was examined through detailed kinetic and thermodynamic studies. The adsorption kinetics data were well-fitted to the pseudo-second-order kinetic model, suggesting chemisorption as the dominant adsorption mechanism. Thermodynamic investigations revealed that the adsorption process was spontaneous (negative Gibbs free energy (ΔG° < 0)) and exothermic (negative enthalpy change (ΔH° < 0)), indicating a favorable interaction between quercetin molecules and the nanocomposite at lower temperatures. Additionally, entropy change (ΔS°) analysis demonstrated decreased randomness at the solid-liquid interface during adsorption. The results confirm that UIO66-NH2@PANI nanocomposite is a promising candidate for the selective adsorption, and recovery of natural antioxidants such as quercetin. These findings contribute to the understanding of the adsorption mechanism and expand the potential applications of metal-organic framework-based nanocomposites in environmental and pharmaceutical fields.

***Keywords:*** Biomolecule quercetin, Kinetics, Nanocomposite, Thermodynamics, Adsorption

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**Missense Nexilin-rs1166698 gene polymorphism may correlate to protein structural disruptions in cardiomyocytes: An *in-silico* study**

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**Abstract**

Nexilin, encoded by the *NEXN* gene, is a vital actin-binding protein that plays a crucial role in maintaining the structural integrity of cardiomyocytes. Disruptions in its structure may contribute to cardiac dysfunction. In this in- silico study, we focused on the structural impact of the rs1166698 single nucleotide polymorphism (SNP) (G>A, Gly181Arg) within the *NEXN* gene. Using bioinformatics tools such as SIFT, PolyPhen-2, and Mutation Assessor, we assessed the Gly181Arg substitution and found it deleterious, indicating potential disruption in protein function. Structural stability analysis performed by I-Mutant, iStable, and MUpro predicted a significant reduction in nexilin's stability due to this mutation, suggesting that the protein may lose its ability to maintain proper mechanical support in heart cells. Furthermore, secondary structure predictions from PSIPRED and GOR-IV showed that the Gly181Arg substitution may alter the folding pattern of nexilin, affecting its structural conformation and potentially leading to functional impairments. As nexilin plays a critical role in anchoring actin filaments, these structural alterations could disrupt the cytoskeletal organization in cardiomyocytes, contributing to arrhythmogenic conditions. Therefore, this study identifies the rs1166698 polymorphism as a potentially significant factor in nexilin dysfunction, warranting further investigation into its role in protein structure and arrhythmia development.

***Keywords:*** Missense single nucleotide polymorphisms, *Nexilin* gene, Protein stability, Protein structure, rs1166698.

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**Effect of asymmetric and symmetric bidentate ligands in the structure of anticancer platinum complexes in cancer treatment**

Mahboube Eslami Moghadam

**Abstract**

To design and synthesize new anticancer Pt drugs, the structure and bioactivity relationship is investigated with the change of ligands and also metal center. The presence of monodentate or bidentate ligands containing symmetric and asymmetric donates, and non-leaving groups, including aliphatic or aromatic compounds can affect the biological activity of these related metallodrugs. In this study, some Pt (II)/Pt (IV) complexes have been prepared where ligand can be NH3, N^N donor like 2,2′-bipyridine, 1,10′-phenanthroline, or R, R diamine-cyclohexane, and also O^O oxalate derivatives, asymmetric N^O amino acid derivatives, and then characterized. The stability, water solubility, and lipophilicity of these complexes were evaluated and compared with clinical Pt drugs such as cisplatin, carboplatin, and oxaliplatin. The *in- vitro* anticancer activities of these compounds were examined against several cancerous cell lines. Data show that due to less steric effect, and the presence of a length aliphatic hydrocarbon chain in the complex structure, more toxicity on cancerous cell lines is expected. Regarding different solubility and lipophilicity behaviors, the accumulation of complexes and clinical Pt drugs in each cancerous cell was investigated. According to data, using bulky ligands leads to lipophilicity modification and less cytotoxic activity, while aromatic groups cause more anticancer ability. Chain and cyclic aliphatic bio-ligands may reduce the bio-efficacy of these compounds. Based on the all-mentioned conclusions, these candidates will be investigated selectively further in *in-vivo* studies and chemotherapy and cancer treatment.

***Keywords:*** Pt (II)/Pt (IV) complexes, Clinical Pt drugs, Cytotoxicity, Solubility, Lipophilicity

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**Gut microbiota and Parkinson's Disease: A double-edged sword**

Fatemeh Miraba,\*, Mitra Pirhaghib, Ali Akbar Sabourya

**Abstract**

Parkinson's disease (PD) is a neurodegenerative disorder characterized by the abnormal accumulation of α-synuclein (α-Syn) in the brain. Recent research highlights the significant role of the gut microbiota, the diverse community of microbes living in the intestines, in modulating α-Syn pathology. This review explores the bidirectional communication along the microbiota-gut-brain axis, focusing on the impact of two gut microbiota metabolites—functional bacterial amyloids (FuBA) and vitamins—on neurodegenerative diseases, particularly PD. FuBA, proteinaceous structures produced by bacteria, contribute to PD pathogenesis by promoting α-Syn aggregation and biofilm formation, which are crucial processes in the development and progression of PD. On the other hand, vitamins, essential micronutrients produced by the gut microbiota, offer neuroprotection through their anti-amyloidogenic, antioxidant, and anti-inflammatory properties. Vitamins such as B vitamins and vitamin K can help reduce oxidative stress, promote neurogenesis, and modulate immune responses, all of which are essential for maintaining brain health. Understanding the complex interplay between the gut microbiota, α-Syn aggregation, and neurodegeneration provides valuable insights into the pathogenesis of PD. Targeting the gut microbiota with therapies aimed at modulating FuBA production or enhancing vitamin synthesis could represent promising avenues for the prevention and treatment of PD. By manipulating the gut microbiome, it may be possible to influence α-Syn aggregation, reduce neuroinflammation, and improve overall brain function in individuals at risk for or diagnosed with PD.

***Keywords:*** Gut microbiota, Functional bacterial amyloids, Vitamin, α-Synuclein, Parkinson’s disease

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**Inhibition of A53T Alpha-synuclein fibrillation by Quercetin and Deep eutectic solvents**

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**Abstract**

The aggregation of the alpha-synuclein protein, particularly the A53T mutant, is strongly linked to neurodegenerative diseases like Parkinson’s disease. Inhibiting alpha-synuclein fibrillation is a promising therapeutic strategy. Quercetin, a bioactive flavonoid known for its antioxidant and anti-aggregative properties, has limited solubility in aqueous environments, hindering its therapeutic use. Recently, deep eutectic solvents (DES) are eco-friendly solvents that can enhance the solubility of hydrophobic compounds. This study investigates the inhibitory effects of quercetin dissolved in DES on A53T alpha-synuclein fibrillation. Using fluorescence microscopy and fibrillation kinetics, we assess the ability of this combination to reduce protein aggregation, suggesting a potential therapy for neurodegenerative diseases. Fluorescence microscopy results demonstrated that quercetin dissolved in DES significantly curbs the fibrillation of A53T alpha-synuclein, as indicated by the reduced formation of fibrils. Furthermore, kinetic analysis revealed that quercetin dissolved in DES prolonged the lag phase of fibrillation from 7 hours to 12 hours, indicating a marked delay in the aggregation process. These findings suggest that quercetin, when combined with DES, can effectively impede the initial stages of protein fibrillation. Our research highlights the therapeutic potential of quercetin in DES for protein misfolding disorders, offering new avenues for research in treating neurodegenerative diseases such as Parkinson’s disease.

***Keywords:*** Alpha-synuclein, Parkinson’s disease, Fibril, Quercetin, Deep eutectic solvents

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**Low expression of tumor suppressor ARID1A correlates with reduced expression of E‑cadherin in colorectal cancer**

Mehran Erfania, Pooneh Mokarramb

**Abstract**

Metastasis is a major cause of death in Colorectal cancer (CRC) patients, and the Epithelial mesenchymal transition (EMT) has been known to be a crucial event in cancer metastasis. Downregulated expression of AT-rich interaction domain-containing protein 1A (ARID1A), a bona fide tumor suppressor gene, plays an important role in promoting EMT and CRC metastasis, but the underlying molecular mechanisms remain poorly understood. Here, we evaluated the correlation between ARID1A expression and EMT‐associated markers, *E-cadherin* and *β-catenin*, in human CRC. We measured the transcription levels of ARID1A, E-cadherin and β-Catenin via real time quantitative PCR (qPCR) in 30 pairs of colorectal cancer tissues and their matched non-tumor adjacent tissues. Interestingly, we found an obvious correlation between the expression of ARID1A and E-cadherin in colorectal cancer tissue samples, however, the correlation coefficient was not perfect (r = -0.526). β-Catenin transcription levels were not found to correlate with ARID1A. Thus, ARID1A downregulation may promote CRC metastasis through decreasing EMT‑related protein E-cadherin and promoting epithelial cell movement.

***Keywords:*** Colorectal cancer, ARID1A, E-cadherin, β-catenin

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**Developing 3D bio-printer for fabrication of microfluidic systems in protein-ligand interaction**

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**Abstract**  
3D bioprinter engineered for the rapid and precise fabrication of microfluidic and millifluidic systems, and designed to enhance studies of protein-ligand interactions. This system integrates microfluidic-optimized nozzles with sub-micrometer precision, enabling swift bio fabrication with biocompatible materials, significantly reducing the time and complexity associated with traditional lithographic or soft lithography techniques. The primary advantage of this bioprinter is its ability to quickly prototype fluidic channels and experimental setups, which facilitates real-time studies of biomolecular interactions in controlled, physiologically relevant conditions. Early experiments demonstrate that the printer can generate intricate fluidic environments faster but lower reproducibility compared to conventional methods. This rapid fabrication process not only accelerates experimental workflows but also enables high-throughput screening applications, such as drug discovery and protein engineering. By simulating protein-ligand binding dynamics more efficiently, this system offers superior versatility for studies in structural biophysics and biochemistry, making it an invaluable tool for advancing biomolecular research.

***Keywords:*** 3D bioprinter, Rapid bio fabrication, Microfluidic systems, Protein-ligand interaction, High-throughput screening

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**Missense *Epoxide Hydrolase 1 -* rs1051740 gene polymorphism may correlate to pre-eclampsia: An *in- silico* study**

Sajedeh Latifia, Abasalt Hosseinzadeh Colagara,\*, Mohammad Karimiana, Mohammad-Taghi Hedayatib

**Abstract**

Epoxide Hydrolase 1 (EPHX1) is a critical biotransformation enzyme that converts epoxides from aromatic compounds' degradation to trans- dihydrodiols that can be conjugated and excreted from the body. *EPHX1* is involved in the metabolism of xenobiotics and steroids and also plays a role in repair following oxidative injury. Mutations in this gene cause pre-eclampsia (PE), epoxide hydrolase deficiency, or increased epoxide hydrolase activity. *In- silico* studies can help to identify the functional role of single nucleotide polymorphisms (SNPs) in the structure and stability of EPHX1 protein and to predict their relationship with PE. This study investigated, missense SNPs of the *EPHX1* gene and their effects on PE. At first, all missense SNPs of the *EPHX1* gene, located on chromosome 1q42.12, were monitored. Missense SNPs with a minor allele frequency (MAF)≥ 0.1 were selected in the NCBI-dbSNP database. The effect of the selected SNP based on functional, structural, and stability aspects of the protein was investigated by the following twelve online software: SIFT, Polyphen-2, PANTHER, SNPs & GO, PhD-SNP, Mutation Assessor, PROVEAN, I-mutant, iStable, MUpro, PSIPRED, and HOPE. Analysis of missense SNP by SIFT, Polyphen-2, PANTHER, and PROVEAN showed that rs1051740 (T>C, Tyr113His), could be a deleterious SNP for the function of *EPHX1*. The prediction of the effects of this SNP by I-mutant, IStable, MUpro, and PSIPRED also showed that substituting Tyr113His may decrease the stability of the protein. On the other hand, The HOPE analysis tool illustrated that the rs1051740 variant could disturb the protein motifs. Our findings suggest thatthe *EPHX1* gene may be involved in the development of PE and rs1051740 may have deleterious impacts on the function of this gene.

***Keywords:*** Epoxide hydrolase 1, Genetic Polymorphism, *In- silico* studies, Missense single nucleotide polymorphisms, Preeclampsia

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**Hydrophobic amino acids functionalized SPION as a powerful tool for insulin nanofibril bio separation**

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**Abstract**

Superparamagnetic iron oxide nanoparticles (SPIONs) have garnered significant interest due to their unique superparamagnetic properties and high surface-area-to-volume ratio, which enhance molecular interactions and facilitate efficient absorption and penetration across various applications. A key feature of SPIONs is their ability to lose magnetization when the external magnetic field is removed, making them ideal for targeted applications and easy removal after use. In this study, SPIONs with an iron oxide core were synthesized via co-precipitation and functionalized with different hydrophobic amino acids to target insulin fibrils formed under stress conditions. Among them, SPIONs functionalized with optimum hydrophobicity were selected. Due to their iron content, these nanoparticles exhibit low toxicity and good biocompatibility with the human body, akin to the iron in hemoglobin. The behavior of the functionalized SPIONs with insulin fibrils was investigated using spectroscopy and fluorescence microscopy. Results demonstrated high selectivity of the SPIONs for insulin fibrils, effectively separating them while exhibiting no such affinity for native insulin. Additionally, the efficacy of SPIONs in the presence of a molecular crowding agent-mimicking the high concentration of fibrillated protein in cellular environments-was confirmed, further highlighting their potential for therapeutic applications.

***Keywords:*** Insulin, Fibrils, Hydrophobicity, Superparamagnetic iron oxide nanoparticles, Amino acid, Bio separation

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**Studying the interaction between four-stranded nucleic acid structures and Actinomycin-D and Berberine**

Niloufar Monzavi, Bita Zamiri\*

**Abstract**

The binding phenomenon between non-canonical nucleic acid structures, specially four-stranded structures such as G-quadruplexes and i-motifs, with small molecules has garnered significant interest in recent years since it can result in the design of therapeutic systems which target unusual nucleic acids involved in disease pathogenesis. This study investigates the binding interaction between Actinomycin D, a chemotherapeutic agent, and Berberine, a natural alkaloid found in plants, with G-quadruplexes and i-motifs formed by four repeats of the *C9orf72* repeat whose expansion is known to cause ALS/FTD. The binding phenomenon has been monitored via UV spectroscopy where we have shown that both Actinomycin D and Berberine exhibit binding with G-quadruplexes and i-motifs reflected in the change in absorbance. Based on the observed hyperchromocity and the dissociation constants calculated, Actinomycin D and Berberine are shown to have slightly higher affinity for the i-motifs formed under acidic conditions.

***Keywords:*** G-quadruplexes, I-motifs, Berberine, Actinomycin D, Drug-DNA binding

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**Simulation of the interaction of a group of inhibitory compounds with the amino domain of the Human T-cell Lymphoma Virus-1 capsid using in-silico methods**

Maryam Bidkhorya, Mitra Kheirabadia,\*, Sakineh Kazemi Noor- aleinia, Maliheh Azadparvarb,\*

**Abstract**

Both Human Immunodeficiency Virus-1 (HIV-1) and Human T-cell Lymphoma Virus-1 (HTLV-1 ) viruses belong to the Retroviridae family. The HTLV-1 virus leads to diseases such as Adult T-cell Leukemia/Lymphoma (ATL) and a progressive neuroinflammatory syndrome called HTLV-1-Associated Myelopathy/Tropical Spastic Parararesis (TSP/HAM), as well as arthropathy in joints and inflammation in the eyes. Additionally, the HIV-1 virus is responsible for causing acquired immunodeficiency syndrome (AIDS). The capsid (P24) is an essential structure for the formation of the complete virus and its replication. Unfortunately, no inhibitory compounds have been proposed to prevent the function of this protein structure in the HTLV-1 virus so far. In the present study, considering the family relationship and certain similarities between the HIV-1 and HTLV-1 viruses, a group of inhibitory compounds that showed suitable effects on the amino domain of the HIV-1 capsid in experimental studies were evaluated on the HTLV-1 capsid using molecular docking and molecular dynamics simulations. These compounds demonstrated effective inhibitory effects on the amino domain of the HTLV-1 capsid. The position of the title in this section is 120 mm from the top of the page or upper edge.

***Keywords:*** Capsid, Inhibitor, Human T-cell Lymphoma Virus-1, Human Immunodeficiency Virus-1

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**Anti Human T-cell Lymphoma virus compounds from fungal metabolites as protease inhibitor; in silico study**

Elahe Shokrollahia, Mitra Kheirabadia,\*, Maryam Bidkhoria, Maliheh Azadparvarb,\*

**Abstract**

There is no curative treatment for patients infected with Human T-cell Lymphoma virus. Human T-cell Lymphoma virus protease plays an important role in activities such as replication cycle and virus maturity. The fungal metabolites as bioactive molecules could potentially be considered as a good source of discovery of new medicines. The aim of the present study was to investigate the inhibitory effect of fungal metabolites on HTLV-1 protease. Twenty fungal secondary metabolites from five different chemical groups were selected based on the inhibitory effects on HIV protease, including Colossolactones, Lanostane type Triterpenoids, Farnesyl Hydroquinone, asterriquinone, Cytochalasins, while indinavir was considered as the control. Human T-cell lymphoma virus protease (PDB code: 3LIN) was selected as the receptor for subsequent computational docking and molecular dynamic simulation study with Autodock and Gromacs, respectively. Results of the docking and molecular dynamic simulation study suggested a favorable binding mode of Colossolactone IV, Colossolactone II, Ganoderiol F, and Schisanlactone to the HTLV protease with respect to indinavir. Analysis of hydrogen bond pattern and RMSF plot revealed a nearly similar ligand-receptor interaction for Colossolactone II and Ganoderiol Fin complex with HTLV protease in comparison with indinavir. Colossolactone II and IV derived from Colossum Ganoderma and Ganoderiol F derived from Ganoderma Lucidum exhibited an anti-HTLV protease effect that has been proposed to be able to be developed as a drug.

***Keywords:*** HTL-V1 protease, inhibitor, Fungal metabolites

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**The volatile compounds α-asarone and β-caryophyllene promote disassembly and dis-aggregation of tau fibrils and aggregates**

Afrooz Anbaraki\*, Arefeh Seyedarabi

**Abstract**

Aggregation and assembly of hyperphosphorylated tau into neurofibrillary tangles is one of the main pathological hallmarks of Alzheimer’s disease (AD) and other tauopathies. Disassembly and disaggregation of tau fibrils and aggregates into the non-toxic tau oligomeric species is recognized as a viable therapeutic strategy. In this study, the effects of the volatile compounds α-asarone (ASA) and β-caryophyllene (BCP) were assessed for their potential to promote the disassembly and dis-aggregation of tau fibrils and aggregates. SDS-PAGE analysis revealed that both ASA and BCP, at certain concentrations, could convert the high molecular weight tau species into their low molecular weight counterparts or monomeric forms. The ThT fluorescence intensities of the pre-formed tau fibrils and aggregates diminished in the presence of ASA and BCP. Furthermore, circular dichroism spectroscopy analysis indicated that ASA and BCP substantially diminished the β-sheet structure of the tau samples, concomitantly increasing the α-helix or random coil contents. Additionally, atomic force microscopy images illustrated that ASA and BCP possess the capacity to convert tau fibrils or aggregates into tau intermediate oligomers. MTT assays indicated that these tau oligomers formed in the presence of ASA and BCP were less toxic to the SH-SY5Y neuroblastoma cells, in comparison to the not-treated positive control sample. All results revealed the potential protective effects of ASA and BCP on tau fibrils and aggregates. Consequently, the volatile compounds ASA and BCP warrant further investigation due to their neuroprotective and therapeutic activities against AD and other tauopathies.

***Keywords:*** α-asarone, β-caryophyllene, Disassembly, Dis-aggregation, Tau protein, Alzheimer’s disease

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**FIRIA: A novel non-invasive technique for breast cancer diagnosis**

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**Abstract**

Functional Infrared Resonance Imaging Assay (FIRIA), a novel non-invasive technique for medical diagnosis, was recently introduced by Jahanfar. In this study, we modeled the FIRIA signals associated with 17 inflammatory factors using Ab Initio Quantum Chemistry software. Our objective was to investigate the potential of FIRIA imaging for diagnosing and monitoring breast cancer using these factors. We obtained the molecular structures of the 17 inflammatory factors from the PubChem databases and the RCSB Protein Bank. After making structural corrections, we utilized the GAMESS software with the DFTB method, applying the OB2W0PT3 parameter. Subsequently, we modeled the FIRIA signals at five different lateral resolutions using Python. Statistical analyses of these 17 signals across all resolutions revealed significant differences in their signal patterns, allowing for clear differentiation between them. Among the modeled FIRIA signals, the most notable variations were found in interferon-gamma, plasmin, thrombin, and tryptase, which had an average RMSD of 4.99. Conversely, the lowest variation was observed in prostaglandin, leukotriene B4, 5-hydroxyeicosatetraenoic acid, and histamine, with an average RMSD of 2.28. Notably, we found that as the resolution increased, the RMSD values and the distinctions between the signals also rose. The findings highlight the high potential of the FIRIA imaging method for diagnosing crucial inflammatory factors and emphasize the feasibility of employing FIRIA for the diagnosis and monitoring of breast cancer and other cancers or diseases where these inflammatory factors hold clinical significance.

***Keywords:*** Radiology, Non-Invasive diagnosis, Breast cancer, Infrared imaging, FIRIA

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**Characterizing minor peaks in DSC thermograms of human serum albumin: Unveiling thermal transition insights**

Bagher Davaeil, Faezeh Moosavi-Movahedi, Ali Akbar Moosavi Movahedi\*

**Abstract**

Previous studies on human serum albumin (HSA) DSC (Differential scanning calorimetry) thermogram have been reports of either two distinct temperature melting point (Tm) or just a single Tm. This study analyses their DSC thermograms by examining the differential thermodynamic behaviour of HSA and HSA-Fatty Acid (HSA-FA) complexes. Notably, minor peaks in the DSC profiles underscore subtle thermal transitions. The minor peak in the DSC thermogram seems to belong to the protein's domain I (DI). Ligand interaction with DI as well as fatty acids (due to their binding site in DI) may facilitate the formation of DI structural interactions. The results obtained, suggest an independent folding of the other two domains, which requires further study to confirmation. The melting temperature (Tm) variations between HSA and HSA-FA reveal significant insights into their stability and interaction mechanisms. These findings highlight the nuanced impact of fatty acid binding on the thermal properties of HSA, offering valuable implications for biochemical and pharmaceutical applications.

***Keywords:*** Human serum albumin , Differential scanning calorimetry, Thermogram of human serum albumin, Minor peak

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**Platinum (IV) prodrugs based on carboplatin with biological approaches to improve drug delivery**

Mahboube Eslami Moghadam\*, Hosein Keivan Shekooh

**Abstract**

Carboplatin is a derivative of cisplatin; with a similar intercellular mechanism and different structure and cytotoxicity. It was approved by the FDA in the 1980s and since then it has been widely used to treat various types of tumors. However, there are serious inconveniences as some patients develop resistance during treatment, limiting the full potential of the drug. Consequently, the discovery of novel metallodrugs with different structural and mechanistic profiles for drug development plays an important role in cancer drug discovery. In this study, a new binuclear carboplatin (IV) derivative was synthesized using diamine as a bridging ligand and then characterized by spectroscopic methods. The reduction behavior in the presence of ascorbic acid was investigated by using electronic absorption monitoring. Regarding *in- vitro* evaluation of this new carboplatin derivative, more toxicity has been shown against MCF-7 cell lines than carboplatin. The cell death mechanism's activity was investigated by using Flow cytometry which determined apoptosis cell death. In addition, DNA interaction and molecular docking display groove binding on sites of the DNA skeleton as a main target in chemotherapy.

***Keywords:*** Binuclear Pt (IV) complex, Anticancer drug, DNA binding, Molecular docking

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**Bio-Based Coatings with Protease Enzymes for Preventing Microorganism Growth on Marine Surfaces**

Saba Ghattavia,\*, Tayebeh Zarei Karyanib, Ehsan Kamrania, Ahmad Homaei

**Abstract**

Marine biofouling on surfaces such as ship hulls and other maritime equipment results in increased fuel consumption, decreased speed, and elevated maintenance expenses. Although chemical antifouling paints are commonly employed to combat this challenge, numerous formulations contain toxic substances detrimental to marine ecosystems. In contrast, protease enzymes present a viable eco-friendly alternative to inhibit the proliferation and accumulation of microorganisms on these surfaces. Protease enzymes were chosen as bioactive antifouling agents due to their ability to degrade proteins, which directly affects the biological integrity of microorganisms. A series of laboratory and field evaluations have shown that coatings exhibiting protease activity effectively hinder the adhesion and growth of bacteria, algae, and various marine organisms on treated surfaces. In conclusion, protease-based bio-coatings not only exhibit significant effectiveness in reducing fouling but also mitigate negative impacts on marine ecosystems, leaving no harmful byproducts upon degradation. So, protease enzymes are a pioneering strategy for the formulation of sustainable antifouling coatings, emphasizing the potential of enzyme-based solutions to alleviate the environmental consequences of antifouling practices within the maritime sector.

***Keywords:*** Bio-Based Coatings, Protease Enzymes, Biofouling, Antifouling, Marine Surfaces

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**Enhanced antitumor activity of the Lapatinib via loading in human serum albumin**

S. Mohsen Asghari

**Abstract**

Triple-negative breast cancer (TNBC) represents a particularly aggressive form of cancer that is notoriously difficult to treat due to the absence of hormone receptors and HER2 expression. Traditional therapeutic strategies have limited efficacy and are often accompanied by significant side effects. Lapatinib (LAP), a tyrosine kinase inhibitor, has shown potential against TNBC; however, its clinical application is hindered by poor aqueous solubility and systemic toxicity. This study explores a novel drug delivery system aimed at enhancing the therapeutic index of Lapatinib through encapsulation with Human Serum Albumin (HSA), a biocompatible and non-toxic carrier recognized for its excellent drug binding capacity. This research aims to improve the therapeutic efficacy and selectivity of Lapatinib for TNBC treatment by employing Human Serum Albumin as a delivery platform. By encapsulating Lapatinib within HSA nanoparticles, the study seeks to enhance its solubility, enable controlled drug release, and reduce the systemic toxicity typically associated with chemotherapy. Lapatinib was incorporated into HSA via hydrophobic interactions, with the resultant HSA-LAP complexes characterized using spectroscopic methods (UV and fluorescence spectroscopy), Atomic Force Microscopy (AFM), and Transmission Electron Microscopy (TEM) to evaluate structural integrity and drug loading efficiency. In- vitro cytotoxicity was assessed using the MTT assay on the 4T1 breast cancer cell line to determine IC50 values. The study also incorporated apoptosis assays (Annexin V/PI staining and caspase activation) and wound healing assays to investigate anti-migratory properties. In vivo efficacy was evaluated using a BALB/c mouse model, measuring tumor growth suppression and survival extensions. Biodistribution studies were facilitated by radiolabeling HSA-LAP with Technetium-99m (99mTc) to observe tumor-targeting abilities. The encapsulation process preserved the structural integrity of HSA with minor conformational changes observed. In- vitro assays demonstrated that HSA-LAP exhibits significantly enhanced anti-proliferative and pro-apoptotic effects on TNBC cells compared to free Lapatinib, with a notable decrease in IC50 values (1.05 µg/mL for HSA-LAP vs. 5.47 µg/mL for LAP). Furthermore, the synergistic combination with VGB3, a VEGFR1/2-targeting peptide, resulted in a dramatic IC50 reduction to 0.2 µg/mL, and a notable increase in apoptosis rates to 50.2%. In the in vivo model, tumor growth was profoundly reduced by 59% with HSA-LAP and 89% when combined with VGB3, together with improved survival rates relative to standard treatment modalities. Biodistribution analysis confirmed preferential uptake of HSA-LAP by tumor tissues, suggesting enhanced targeting and retention capabilities. These findings affirm the potential of HSA as a highly effective delivery system for Lapatinib, significantly augmenting its anticancer potency against TNBC. The research highlights the merits of using HSA in drug formulation, offering optimized delivery profiles that mitigate systemic toxicity. Moreover, the impactful results of the combined therapy with VGB3 warrant further exploration and development, potentially offering a transformative approach in treating aggressive breast cancer subtypes.

***Keywords:*** Lapatinib, Human serum albumin, Triple-negative breast cancer, Drug delivery systems, Combination therapy

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**Stabilization of recombinant α-amylase using a cellulose/gold hybrid nanosupport**

Mozhgan Razzaghia, Ahmad Homaeia,\*, Roohullah Hemmatib, Dariush Saberic, Soudabeh Kavousipourd

**Abstract**

α-Amylase is one of the most widely used commercial enzymes across various industries. In this study, the gene encoding α-amylase from Bacillus aquimaris MKSC 6.2 (BaqA) was subcloned into the expression vector pET28a(+) and successfully expressed in E. coli BL21 (DE3). The synthesis of a cellulose nanocrystals/gold nanoparticles (CNC/AuNPs) hybrid was accomplished using a hydrothermal treatment without toxic chemicals. Recombinant BaqA was covalently attached to a cysteine-modified nanosupport through a Schiff base reaction via glutaraldehyde linkages. The successful synthesis of the designed nanohybrid and the enzyme stabilization process were confirmed by Fourier Transform Infrared Spectroscopy (FT-IR), Dynamic Light Scattering (DLS), intrinsic fluorescence, Ultraviolet-Visible (UV-Vis) spectroscopy, Field Emission Scanning Electron Microscopy (FESEM), and Energy-Dispersive X-ray Spectroscopy (EDX) techniques. Free α-amylase exhibited maximum activity at pH 10 and a temperature of 70 °C. The optimal temperature for the immobilized enzyme increased to 80 °C, while the optimal pH remained unchanged. This catalytic platform significantly enhanced chemical and thermal stability as well as enzyme stability under critical pH conditions. After a four-week storage period, the immobilized α-amylase retained 67.5% of its initial activity, in contrast to the free α-amylase, which retained only 17% under the same conditions. Following 11 consecutive uses, the immobilized enzyme retained 75% of its initial activity. Based on the obtained results, the produced nanoenzyme could serve as a suitable candidate for industrial applications under harsh and critical conditions.

***Keywords:*** α-Amylase, Recombinant, Hybrid nanoparticles, Stability, Immobilization, Reusability

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**Biochemical pathways in *Penaeus vannamei* protease stabilization via zinc sulfide** **nanoparticle mediation**

Mozhgan Razzaghia, Ahmad Homaeib,⁎, Elaheh Mosaddeghc

**Abstract**

Zinc sulfide (ZnS) nanoparticles have gained extensive attention in biomedical and biotechnological research due to their biocompatibility and non-toxic properties, positioning them as ideal platforms for various therapeutic and industrial applications. This study investigates the potential of ZnS nanoparticles synthesized via chemical precipitation as a support for immobilizing protease enzyme derived from *Penaeus vannamei* shrimp. Immobilizing enzymes on nanoparticle surfaces often leads to improved stability and performance, addressing common challenges in enzyme applications, such as decreased catalytic efficiency over time. Advanced characterization techniques, including Fourier-transform infrared (FT-IR) spectroscopy, ultraviolet-visible (UV-Vis) spectroscopy, dynamic light scattering (DLS), and transmission electron microscopy (TEM), were employed to comprehensively assess the ZnS nanoparticles before and after enzyme immobilization. These methods provided insights into particle size, surface structure, and morphological changes post-immobilization, which are essential for optimizing immobilized enzyme functionality. Results demonstrated a significant enhancement in the thermal and long-term stability of the immobilized protease enzyme compared to its free form. Additionally, immobilization improved the enzyme's resistance to extreme pH levels, advantageous for industrial applications. Notably, the immobilized enzyme exhibited an increase in optimal operating temperature, while kinetic parameters remained largely unaffected, indicating minimal loss in catalytic efficiency. These findings suggest that ZnS nanoparticle-supported enzymes have promising potential for diverse industrial applications, offering enhanced enzyme stability and resilience under challenging operational conditions.

***Keywords:*** Zinc sulfide nanoparticles, Protease enzyme, Immobilization, Stability, Catalytic efficiency

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**Comparison of bio-optical properties of hypoxylonol compound using density functional theory and molecular docking**

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**Abstract**

This article investigates the optoelectronic and biological properties of Hypoxylonol-F. The importance of this drug lies in its potential biological activities, which include antiviral, antibacterial, and anticancer properties. Electronic and optical calculations were performed using Density Functional Theory and the Full-Potential Linearized Augmented Plane Wave method. Additionally, molecular docking was conducted to investigate the inhibitory effect of this compound on Human Immunodeficiency Virus-1 and Human T-cell Lymphoma Virus-1 proteases. Electronic calculations show that Hypoxylonol-F is an insulator with an indirect band gap of about 2.03 electron volts, indicating the stability of the compound. The p orbitals of carbon atoms play an active role at the Fermi level and participate in bonding with other compounds. This compound exhibits high absorption in the Extreme ultraviolet region. It is also shown that the binding between the Hypoxylonol-F ligand and HTLV protease occurs at a lower energy. The binding energy obtained from docking calculations is consistent with the Density Functional Theory density of states diagram.

***Keywords:*** Human Immunodeficiency Virus-1, Human T-cell Lymphoma Virus-1, Hypoxylonol-F, Density functional theory, Molecular docking, Electronic and optical properties

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**Microfluidic chips efficacy to induce bovine serum albumin aggregation at room and physiological temperature**

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**Abstract**

Recently Microfluidic chips gained so much attentions and are considered as valuable tools for studying protein aggregation, allowing investigation into the effects of various variables on protein aggregation, including chemical and physical factors. This study examined bovine serum albumin (BSA) aggregation in both a conventional vial system and a microfluidic chip. While BSA aggregation in vials has been well-characterized, our focus was on exploring temperature-dependent aggregation within the microfluidic environment. By employing biophysical techniques, we demonstrated the formation of amyloid-like BSA aggregates at physiological pH across a range of temperatures: 70°C (above the melting point, *T*m = 65°C), 37°C, and 25°C. Notably, unlike the vial system where aggregation was primarily observed at elevated temperatures, the microfluidic chip facilitated aggregation even at room and physiological temperatures, with more pronounced aggregation at 37°C. This work provides valuable insights into the mechanisms underlying protein aggregation and highlights the potential of microfluidic technologies for studying complex biological processes.

***Keywords:*** Amyloid-like structures, Microfluidic chip, Physiological temperature, Bovine serum albumin aggregation

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**Application of click chemistry for protein modification: HSA-biopolymer scaffold fabrication via bioorthogonal reaction**

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**Abstract**

In this study, we explore the potential of click chemistry for protein modification and the development of novel protein-based materials. For the first time in Iran, we employ a copper-catalyzed azide-alkyne cycloaddition (CuAAC) click reaction to synthesize a new protein-biopolymer scaffold using a covalent bioconjugation strategy. We have successfully designed and manufactured this innovative scaffold by integrating protein engineering, click chemistry and polymer science. The scaffold, composed of natural and synthetic polymers, displays biocompatibility, mechanical stability, and tunable functionality, making it a promising candidate for various applications. These properties can be tailored by modifying the composition and architecture of the scaffold, offering a versatile platform for bioengineering applications such as drug delivery, tissue engineering, and biosensing. Our findings demonstrate that the CuAAC click reaction is an effective tool for fabricating protein-based materials with potential applications in biotechnology and medicine. The protein-biopolymer scaffold developed in this study opens new avenues for exploring click-mediated proteins with promising applications. This research highlights the potential of this approach in advancing the field of protein-based materials, paving the way for further innovation and the development of novel biomaterials with enhanced properties and functionalities.

***Keywords:*** Human serum albumin, Biopolymer, Click chemistry, Copper-catalyzed azide-alkyne cycloaddition

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**Targeted colorimetric assay for rapid detection of *moraxella catarrhalis* through spectroscopic analysis**

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**Abstract**

*Moraxella catarrhalis (M. catarrhalis)* is a β-lactam resistant respiratory pathogen posing diagnostic challenges and lacks an available vaccine. This study introduces a rapid molecular and colorimetric assay, which is essential for timely diagnosis and improved infection management. The *ompCD* gene, encoding an outer membrane protein, was targeted as a nucleobiomarker in *M. catarrhalis* and compared with 9 other Gram-positive and Gram-negative bacteria. *M. catarrhalis* and the other strains were cultured in BHI and TSB media at 36°C, respectively. Following incubation, DNA was extracted using the boiling method and PCR-amplified with specific primers. The amplicons were confirmed by gel electrophoresis and assessed using a colorimetric method through spectrophotometry with the Neutral Red indicator. The sensitivity of the method was evaluated using a decimal serial dilution of the extracted *M. catarrhalis* DNA. *M. catarrhalis* was harvested at the stationary phase after 48 h, while the other strains were harvested after overnight incubation. Gel electrophoresis of the PCR amplicons revealed a distinct band in the range of 200-300 bp specific to *M. catarrhalis*, which was not observed in the other strains. In the colorimetric assay, *M. catarrhalis* exhibited a distinct orange-red color, contrasting with the deep red observed in the other strains. Optical density (OD) was measured at the range of 400-700 nm. Spectroscopic analysis revealed distinct peaks at 450 nm and 570 nm for *M. catarrhalis*, showing higher absorbance at 450 nm (0.358) and lower absorbance at 570 nm (0.249). In contrast, the other strains exhibited the opposite pattern, with lower absorbance at 450 nm and higher absorbance at 570 nm. The specificity for the tested bacteria was 100 percent. The sensitivity of the method was measured as 0.05 ng/μL. In conclusion, the colorimetric assay for *M. catarrhalis* detection is more effective than conventional methods, enabling the possibility of faster therapeutic prescriptions.

***Keywords:*** Moraxella catarrhalis, Respiratory pathogen, ompCD gene, Colorimetry detection

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**Identification of Potential COVID-19 Mpro inhibitors through covalent drug docking, molecular dynamics simulation, and MMGBSA calculation**

Mohammad Hossein Haghir Ebrahim Abadi, Yahya Sefidbakht\*

**Abstract**

The viral main protease (Mpro) is a key drug target due to its integral role in the life cycle of SARS-CoV-2. Given the urgent need for effective therapeutics against COVID-19, extensive research has focused on the development of inhibitors targeting this enzyme. This study focuses on the exploration of covalent docking for Mpro inhibition. Using computational methods, the interactions between potential inhibitors and SARS-CoV-2 Mpro are investigated. Using protein structures (7JKV and 7TDU), fragment-based ligand selection and covalent docking via SeeSAR were performed. Pharmacokinetic properties, toxicity assessments using SwissADME and molecular dynamics simulations were performed using GROMACS. Molecular dynamics simulations were performed and parameters such as RMSD, RMSF, and MM/GBSA were analyzed for two specific ligands. These inhibitors exhibit pharmacological properties that may affect drug interactions and metabolism in vivo. In addition, the toxicity profiles of covalent ligands highlight complex interactions across physiological systems and underscore the need for comprehensive safety evaluations prior to therapeutic considerations.

***Keywords:*** COVID-19, Main protease (Mpro), Computational drug design, Covalent drug design

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**The study of salt concentration effect on α-synuclein fibril structure in the presence of an electric field**

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**Abstract**

Aggregation of the intrinsically disordered protein α-synuclein is the primary cause of Parkinson's disease and related neurodegenerative disorders. Multiple studies have shown that electric fields at various voltages have significant effects on the secondary structure of proteins. Moreover, the influence of salt concentration is crucial in the aggregation process of α-synuclein. In this study, we conducted two all-atom molecular dynamics simulations for 60 nanoseconds on α-synuclein fibrils to elucidate the structural features of protein fibrils under the influence of an electric field (0.4 V/nm) and a low salt concentration (50 mM). We prepared two systems under the effect of an electric field and introduced salt concentration to one of them. This comprehensive approach provided valuable insights into the role of salt concentration and electric fields in shaping the structure of α-synuclein fibrils. The results indicate that the number of hydrogen bonds decreases under the influence of an electric field, suggesting instability of the beta structures, which are crucial for fibril consistency. Additionally, the number of helices and coils increases. Nevertheless, the ratio of helix to coil under the combined effect of salt and an electric field is higher than that observed without the application of salt concentration. Overall, this study has the potential to enhance our understanding of the molecular mechanisms underlying neurodegenerative diseases and may contribute to the development of novel therapeutic strategies targeting α-synuclein fibrils.

***Keywords:*** Electric field, Salt concentration, α-Synuclein, Aggregation, Parkinson’s disease

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**Conformational changes of αB-crystallin upon the effect of its glycation by methylglyoxal**

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**Abstract**

αB-crystallin is one of the main types of soluble proteins in the eye lens, which in addition to its structural role also has chaperone activity. Due to its long lifetime, this protein is susceptible to many post-translational modifications, and mong them, non-enzymatic glycation of αB-crystallin is particularly important because it is involved in age-related and diabetic cataracts. The concentration of methylglyoxal in human blood plasma and lens is approximately 80 nM and 2 μM, respectively. In addition, its concentration increases several-fold in hyperglycemia caused by diabetes. Methylglyoxal is converted to D-lactate in the lens by the enzyme glyoxalase 1, but the activity of this enzyme decreases with age. This study investigated the effect of methylglyoxal on the conformation, aggregation, and stability of αB-crystallin using various techniques such as fluorescence, UV-vis, and SDS-page. The results show that glycation of αB-crystallin with methylglyoxal leads to partial unfolding of the αB-crystallin and causes cross-links between the amino acids arginine and lysine of αB-crystallin by forming advanced glycation end products (AGEs). The result of these cross-links is the formation of high molecular weight protein aggregates. These aggregates are much more stable than native αB-crystallin due to their covalent cross-links. The increase in Tm of the protein with increasing concentration of methylglyoxal also indicates the stability of the protein aggregates. The final result of this modification can lead to αB-crystallin aggregation and opacity of the eye lens.

***Keywords:*** αB-crystallin, Glycation, Aggregation, Methylglyoxal

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**Fluorescence investigation on the interaction of Phyto-synthesized zinc oxide nanoparticles with bovine serum albumin**

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**Abstract**

The environmentally friendly synthesis of nanoparticles has garnered significant interest due to the increasing need for safe, cost-effective, and sustainable technologies in nanomaterial production [1]. This study presents a novel and eco-conscious method for synthesizing zinc oxide nanoparticles (ZnO NPs) utilizing *Ficus religiosa* leaf extract as a renewable, non-toxic, and effective stabilizer. The successful formation of the biosynthesized ZnO NPs was confirmed through UV–Vis spectroscopy, X-ray diffraction (XRD), and field emission scanning electron microscopy (FE-SEM). Furthermore, a fluorescence-based technique was developed for the rapid and straightforward assessment of the interaction between the Phyto-synthesized ZnO NPs and bovine serum albumin (BSA), a crucial carrier protein, under simulated physiological conditions at pH 7.4. This method is characterized by its ease of use, reliability, and practicality [2]. The experimental findings demonstrated that the intrinsic fluorescence of BSA could be quenched by the phyto-synthesized ZnO NPs. The Stern-Volmer plot exhibited a nonlinear trend with an initial upward curvature, likely resulting from a combination of static and dynamic quenching mechanisms [3]. The quenching constants and binding parameters, including binding constants and the number of binding sites, were determined using the fluorescence quenching data. Additionally, synchronous fluorescence spectroscopy indicated slight alterations in the local polarity surrounding the tryptophan and tyrosine residues during their interaction with the ZnO NPs [4]. The biological implications of this research are significant, as albumin functions as a carrier for various ligands. Consequently, this study could offer a new approach to investigate the biological toxicity of green synthesized ZnO NPs at the protein level.

*Keywords:* Green synthesis, Zinc oxide nanoparticles, Bovine serum albumin, Fluorescence spectroscopy

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**Release of quercetin drug using Chitosan-alginate nano capsules**

Vahideh Abdi, Zahra Ghasemi\*, Iman Sourinejad

**Abstract**

Quercetin is a flavonoid, abundantly present in edible plants, fruits and vegetables and has gained considerable interest for its antioxidant property. In spite of its wide spectrum of pharmacological properties quercetin suffer hindrances in clinical applications due to its low aqueous solubility, low bioavailability and instability in the physiological medium. One approach to overcome these problems is to encapsulate quercetin in carriers formed from naturally occurring polysaccharides. Polysaccharides are biopolymers that are widely applied for biomedical and pharmaceutical purpose. Among such polysaccharides, chitosan and alginate have been widely used as particulate carriers for encapsulation and controlled release of bioactive compounds. Alginate and chitosan polysaccharides have been widely used in drug delivery systems because of their biodegradable, biocompatible, non-toxic and bio adhesive properties. Alginate-chitosan nano capsules protect the encapsulated drug from enzymatic degradation, deliver the drug to the target organ, and permit controlled release of the drug. There have been wide ranging studies on drug delivery systems up to date. Among them, the fabrication of nano-size drug delivery systems and utilizing them for the effective and controlled delivery of drugs is an emerging and promising field of research. According to the findings of this study, manufactured nano capsules can be considered as a suitable option for intelligent drug delivery.

***Keywords:*** Quercetin, Chitosan-alginate, Nano capsule, Drug delivery

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**Potential of neratinib and other compounds as tyrosine kinase inhibitors in cancer treatment: Virtual screening and molecular dynamics analysis**

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**Abstract**

Cancer is a life-threatening ailment characterized by the uncontrolled proliferation of cells. Because cancer is not just a single disease, it is unlikely that there will ever be a single cure for it. At present, no proper therapy is available for the disease, and it is increasing day by day with a high mortality rate. Therefore, the need for drugs to combat this disease has increased. Worldwide collaborative efforts from scientists are underway to determine cancer and reduce mortality rates. Tyrosine kinase inhibitors (TKIs) are widely used in tumor treatment. The screened compounds were followed for SP docking, Extra precision (XP) docking, MM-GBSA analysis, induced-fit (IFD) docking, and MD simulation The absorption, distribution, metabolism, excretion, and toxicity (ADMET) properties of all compounds were analyzed and a final selection was made based on the Lipinski rule of five. Then, ADME/T profiles were determined to validate the pharmacokinetics and pharmacodynamics properties of the hit compounds. the promising ADME properties of the selected compounds emphasize their potential as attractive candidates for cancer treatments. The ligand neratinib revealed the highest docking score of -12.154 kcal/mol. To further validate the interactions of top-scored receptors and ligands, a molecular dynamics study of 4 ns was carried out. This indicated that the protein-ligand complex was stable throughout the simulation period, and minimal backbone fluctuations ensued in the system. Post-MM-GBSA analysis of molecular dynamics data showed a free binding energy of -68.391 kcal/mol. This molecule may emerge as a promising ligand against cancer and thus needs further detailed investigations. These virtual investigations revealed four compounds having binding free energies of − 68.391, − 68.314, − 54.021, and − 51.873 kcal/mol respectively as calculated by the MM-GBSA method. The MD simulation studies confirmed the stability of protein-ligand complexes.

***Keywords:*** Absorption, distribution, metabolism, excretion, and toxicity (ADMET), MM-GBSA, [Molecular dynamics](https://www.benthamdirect.com/search?value1=%27molecular+dynamics%27&option1=pub_keyword), [Molecular docking](https://www.benthamdirect.com/search?value1=%27Molecular+docking%27&option1=pub_keyword)

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**Optimization of quercetin concentration for studying liquid-liquid phase separation**

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**Abstract**

Liquid-liquid phase separation (LLPS) of proteins is crucial for understanding the mechanisms of protein aggregation. LLPS acts as an initial stage in protein aggregation, enabling proteins to transition from a uniform solution to distinct phases or concentrated droplets. This study examines the effects of varying concentrations of quercetin on the structural properties of bovine serum albumin (BSA) and aims to identify optimal conditions for studying LLPS. To determine suitable quercetin concentrations for analyzing BSA's structural integrity and interactions, we utilized fluorescence spectroscopy and circular dichroism (CD) spectroscopy. Changes in the protein's secondary structure were evaluated using CD in the far-UV range, while alternations in its tertiary structure were examined through the intrinsic fluorescence of tryptophan and ANS (8-anilino-1-naphthalenesulfonic acid). Our findings reveal that quercetin concentrations of 4.5 μM and 45 μM have minimal effect on the tertiary structure of the BSA monomer, establishing these concentrations optimal for LLPS studies. Additionally, the role of these concentrations can be explored in the context of protein droplet formation during phase separation and the resulting aggregates.

***Keywords:*** Liquid-liquid phase separation, Liquid droplet, Quercetin, Bovine serum albumin

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**Towards controlling calcium spikes, as the cellular clock, by magnetic fields**

Seyed Peyman Shariatpanahi\*, Bahram Goliaei, Ali Same, Sharzad Hadichegini

**Abstract**

Calcium spikes in cells function analogously to clock signals in microprocessors, regulating cellular activities through their frequency. These spikes, controlled by signaling pathways, particularly in the microenvironment between mitochondria and the endoplasmic reticulum, dictate the timing of gene expression and other cellular processes. High-frequency calcium spikes accelerate cellular functions, driving rapid gene expression and metabolic activities. Conversely, in aging cells, the frequency of calcium spikes diminishes, leading to a deceleration of cellular processes, akin to a slower clock speed in microprocessors. This reduction in spike frequency effectively slows down the cellular &quot;time,&quot; impacting the overall functionality and efficiency of the cell. Understanding the dynamics of calcium spikes and their frequency offers insights into cellular aging and potential therapeutic targets for age-related cellular dysfunctions such as diabetes. This knowledge can help develop strategies to maintain cellular function and mitigate the effects of aging on cellular processes. Calcium spikes within a cell result from a positive feedback mechanism in the IP3 channels on the endoplasmic reticulum. These channels are primarily controlled by reactive oxygen species (ROS), which are mostly produced in the mitochondria. Additionally, the frequency of calcium spikes can be modulated by external magnetic fields, which directly affect ROS production in mitochondria. Our studies have shown that electromagnetic fields can influence ROS levels, thereby impacting calcium signaling pathways. This modulation offers potential therapeutic avenues for controlling cellular processes and addressing diseases associated with calcium signaling dysregulation. Over the past few years, we have conducted convergent research on calcium spike dynamics and the effects of ROS and magnetic fields on this phenomenon. The results show a promising capability for controlling calcium spikes, effectively acting as the cellular clock.

***Keywords:*** Towards Controlling Calcium Spikes, as the Cellular Clock, by magnetic fields

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**Multispectral, molecular docking and molecular dynamic simulation studies of DNA binding of a β-ionone-derived ester**

Majid Mahdavi

**Abstract**

β-Ionone is the end-ring counterpart of β-carotenoids, which are widely found in fruits and vegetables. In this research, interaction between DNA and a β-Ionone-derived ester, *(E)-4-(2,6,6-trimethylcyclohex-1-enyl) but-3-en-2-ylpyrazine-2-carboxylate* (4-TM. P), have been elucidated by various methods, such as ultraviolet-visible spectroscopy, fluorescence assays, viscosity measurements, molecular docking, and dynamic simulation. Analyses of multi-spectroscopy and viscosity assays strongly implies the groove binding of 4-TM. P to Ct-DNA. The fluorescence emission spectra of 4-TM. P values for the different Ct-DNA concentrations at 298 K showed an interaction between 4-TM. P and Ct-DNA, leading to quenching of the intrinsic fluorescence of 4-TM. P. Moreover, a fluorescence enhancement indicated a static process characterized by complex formation between 4-TM. P and Ct-DNA. The viscosity measurements demonstrated the binding mechanism between 4-TM. P and Ct-DNA because it offers unequivocal evidence of their interaction. Molecular docking simulation using AutoDock4.2 revealed that 4-TM. P was placed at the minor groove of the B-DNA, confirming the above experimental results. The dynamic stability of the complex was also confirmed using molecular dynamic simulation analyses.

***Keywords:*** β-Ionone, DNA interaction, Docking, Dynamic simulation

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**Synthesis of Tartrate-Based Nanoporous MOF for Palbociclib Delivery**

Mergan Haghshenas, Maryam Tohidia, Banafsheh Rastegari

**Abstract**

The synthesis of biocompatible nanoporous metal-organic framework (MOF) based on tartrate was performed in the presence of protein and palbociclib (Pal) as a template for the biomineralization process and, an anticancer drug, respectively. The synthesis of MOF was completed in a single step at room temperature in aqueous media. To the best of our knowledge, this is the first report about the one-pot encapsulation of Pal in a biocompatible framework in a green solvent. This method enables high Pal loading in the framework structure (ca. 86%) at a short time of 15 min. The effect of protein concentration was investigated on the size, morphology, and crystallinity of the synthesized structures. The products were characterized with scanning electron microscopy, X-ray diffraction, Fourier transform infrared, and UV-vis spectroscopy techniques. The release rate of Pal from MOF was studied at different pH values. In- vitro drug release of Pal was slower in alkaline medium (pH 7.4) compared to acidic medium (pH 5.5). The cytotoxicity of different structures was evaluated by the standard 3-(4,5 dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) assay on the two cell lines (NIH/3T3 (normal cell), and B16 (cancer cell)). These results suggested that the designed drug loaded MOF can have a promising effect on the treatment of cancer cells.

***Keywords:*** Bio Metal-Organic Framework (MOF), Drug delivery, Cancer, Palbociclib

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**Alpha amylase inhibitory plants**

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**Abstract**

Alpha-amylase is a low molecular weight endo hydrolase enzyme that catalyzes the hydrolysis of starch and, ultimately, the production of glucose. This enzyme is considered one of the key enzymes and its inhibition can play a significant role in the treatment of diabetes. By controlling the catalytic activity of this enzyme, we can expect a reduction in glucose production in the post-meal phase, which can be a therapeutic advantage for people with diabetes. Today, the importance of using natural sources as inhibitors of alpha-amylase enzyme compared to chemical inhibitors has been much considered due to fewer side effects. Plant’s inhibitory effects on this enzyme can be attributed to their secondary metabolites, such as phenolics, terpenoids, flavonoids and coumarin phytochemicals. Some plant extracts, especially extracts rich in proanthocyanidin, can inhibit enzymes such as alpha-amylase, which can help control and treat diabetes.

***Keywords:*** Alpha-amylase, Inhibition, Herbal extract, Diabetes

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**Analysis of Binding Pattern Changes of Regulatory Factors with Different Alleles in FAS Gene Polymorphism**

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**Abstract**

Many non-coding single nucleotide polymorphisms (SNPs) are located in regulatory regions such as promoter regions and hence can affect gene expression by changing the binding affinity of regulatory proteins. FAS is a cell surface receptor that, due to the interaction with its ligand (FAS Ligand), initiates the cell death signal cascade, and its disruption induces tumorigenesis. The aim of this study is to investigate the change of binding pattern of different transcription and splicing factors with allelic change of Fas gene polymorphisms by in silico method.

Materials and methods: For this analysis, online software such as AliBAba, Spliceaid 2 and Haploreg were used. Promoter polymorphisms of rs2234767 and rs1800682 of Fas gene were investigated.

Results: The results show that due to the change of nucleotide A to G in the -670 A/G polymorphism of the FAS gene, the proteins CFOS, GATA2, CEBPB, TBP, POL2 and STAT3 become binding. Also, due to the change of the G nucleotide to A in the 1377 G/A polymorphism of the FAS gene, EBF1, OCT2 and POU2F2 proteins are binding. SRp55, which is one of the most common splicing factors, is able to bind to the FAS gene by allelic change in the rs1800682 polymorphism.

Discussion: Changes in the binding ability of regulatory proteins such as transcription and splicing factors can increase our better understanding of the molecular mechanisms that lead to various diseases and be considered as a biological marker or therapeutic target in the future.

***Keywords:*** *FAS* gene, Polymorphism, rs1800682, Transcription factor

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**Immobilization of alkaline protease PersiProtease1 by Cross-Linked Enzyme Aggregates (CLEA) method**

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**Abstract**

Proteases are essential enzymes extensively employed in numerous industrial processes, including food production, detergent manufacturing, pharmaceuticals, and leather processing, where they play a pivotal role in enhancing efficiency, product quality, and sustainability by facilitating the breakdown of proteins under diverse conditions. Nonetheless, the industrial use of proteases is constrained by challenges such as reduced stability under harsh conditions, high production costs, and difficulties in enzyme recovery and reuse, which hinder their long-term and cost-effective application in various sectors. Enzyme immobilization has proven to be a viable strategy to address many of these challenges. Among different immobilization techniques, the Cross-Linked Enzyme Aggregates (CLEA) method stands out for enhancing enzyme stability through cross-linking enzyme molecules with bifunctional agents, without the need for external carriers or coatings. In this study, the alkaline protease PersiProtease1 was immobilized using the CLEA method. The immobilization involved using 55% (w/v) saturated ammonium sulfate as the precipitant and 25% (w/v) glutaraldehyde as the cross-linker, maintaining the reaction at 25°C for 17 hours. The immobilized enzyme exhibited a stability increase of over two-fold compared to the free enzyme, demonstrating the CLEA method's efficacy in enhancing enzyme performance. These findings highlight promising applications in biodiesel production, wastewater treatment, textile and leather processing, detergent formulation, and pharmaceutical industries.

***Keywords:*** Cross-linked enzyme aggregates, Enzyme immobilization, Glutaraldehyde, Industrial application, Protease

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**Structural insights into kinase domain of RIP1**

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**Abstract**

The receptor-interacting protein kinase 1 (RIP1) plays a crucial role in cellular signaling pathways, particularly in regulating apoptosis and necroptosis [1]. Understanding the structural dynamics of kinase domain of RIP1 is essential for elucidating its functional mechanisms and therapeutic potential [2, 3]. This study aims to compare the structural characteristics of the native RIP1 kinase domain with the S166A mutant variant, utilizing molecular dynamics simulations (Gromacs-2019.2) to analyze key biophysical properties. Results reveal significant differences in the root mean square deviation (RMSD), radius of gyration (Rg), and root mean square fluctuation (RMSF) between the native and mutant forms. The RMSD analysis indicates a more stable conformation for the native kinase domain, while the S166A mutant exhibits increased fluctuations, suggesting a potential loss of structural integrity. The S166A mutation results in decreased hydrogen bond numbers (H-bonds) and a lower Rg value, suggesting a more compact and stable conformation than the native structure. Additionally, the analysis of the solvent-accessible surface area (SASA) further corroborates these findings, indicating enhanced exposure of hydrophobic regions in the mutant. In conclusion, our findings provide valuable insights into the structural implications of the S166A mutation in the kinase domain of RIP1. These results underscore the importance of specific residues in maintaining the stability and functionality of the kinase domain, offering potential avenues for targeted therapeutic strategies in diseases associated with dysregulated RIP1 activity.

***Keywords:*** RIP1, Kinase Domain, MutantS166A, MD simulation

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**Targeted treatment of the effective herbal ingredient papaverine in the ERK-MAPK signaling pathway of breast cancer cells *in-silico* and *in- vitro***

Fatemeh Hajipour

**Abstract**

Breast cancer is a deadly disease that causes the death and disability of hundreds of women around the world every year. The poppy plant contains important medicinal alkaloids, such as morphine, codeine, and papaverine, which have high economic value in the pharmaceutical industry. So far, different strategies have been used to commercialize their extraction. The aim of this research was to investigate the proliferative or inhibitory effect of the active substance papaverine on breast cancer cells. In order to carry out this research, three proteins—MEK2, MEK1, and BRAF—were used. To determine the effective dose of the researched herbal substance, the MTT test was performed on the cell lines. The samples were then diluted with MTT dye solution, mixed, and incubated. Real-time PCR is a practical method for the amplification of cDNA extracted from RNA, and it was used in this research. The purity of the RNA sample was checked by optical absorption or spectrophotometry. The melting curve and the duplication of each gene were plotted and checked. Docking methods were used to investigate the composition of papaverine on MEK2, MEK1, and BRAF. After the docking, the three-dimensional structure of the ligand-receptor complex and its binding type were studied. Graphs were created and entered into bioinformatics statistical calculations. This research showed that the active ingredient papaverine in poppy plant can play a therapeutic role in the ERK-MAPK pathway of breast cancer cells.

***Keywords:*** Breast Cancer, MEK1, Papaverine, ERK-MAPK

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**Potential of organometallic complexes in medicinal chemistry**

Sedigheh Abedanzadeh

**Abstract**

Medicinal inorganic chemistry is an interdisciplinary research area that has grown primarily due to the serendipitous discovery of Cisplatin, a platinum-based anticancer drug developed in the late 1960s. In the last decades, a significant amount of research has been carried out designing and discovering new metallodrugs with lower level of limitations. To achieve a new metal complex with improved biological activity and decreased cytotoxicity, both the metal center and the surrounding organic ligands play key roles. Organometallic complexes, chemical compounds containing at least one direct metal-carbon bond, are well known for their many applications in various fields of research including medicinal chemistry. Organometallic complexes with specific characteristics including structural diversity, possibility of ligand exchange, redox and catalytic properties have recently gained much attraction for medicinal purposes. The distinct physiochemical properties of organometallic complexes along with the presence of strong metal-carbon σ-bond, have made them valuable in therapeutic studies. They are promising candidates to enhance the effectiveness of treatments, broaden their range of action, reduce adverse effects, and prevent resistance. Herein, we highlight the important role of organometallic metal complexes in metallodrug design.

***Keywords:*** Metallodrug, Cyclometalated complex, Bioinorganic chemistry, Structural diversity, biological activity

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**Clustered regularly interspaced short palindromic repeats/CRISPR-associated protein-based impedimetric biosensor for detection of SARS-CoV-2**

Mohammad Behnam Rad, Hedayatollah Ghourchian\*

**Abstract**

In this study, we designed a clustered regularly interspaced short palindromic repeats/CRISPR-associated protein (CRISPR/Cas)-based impedimetric biosensor which operates as follows: The 20-mer poly adenine probes are immobilized on the surface of a gold working electrode, and their free thiolated tails are bound with gold magnetic nanoparticles. We designed a single guide RNA (sgRNA) targeting the conserved region of ORF1ab in the SARS-CoV-2 virus. In the presence of target, the sgRNA binds to the target sequence and activates Cas12a. The collateral nuclease activity of Cas12a, once activated, cleaves the immobilized probe. Consequently, the gold magnetic nanoparticles are released and adsorbed onto the gold electrode surface using an external magnet. The absorption of nanoparticles increases the physical surface area of the gold electrode, facilitating redox ion electron transfer, and decreasing the charge transfer resistance. We utilized a low-cost polytetrafluoroethylene setup equipped with three electrodes for the impedimetric detection of target nucleic acid. The amplification-free setup demonstrates high specificity and sensitivity for detecting SARS-CoV-2 samples with a detection limit of 8.3 fM and a linear responce range for concentrations from 0.7 to 175 pM. Due to its simplicity and low reagent cost, this electrochemical biosensing platform, utilizing CRISPR/Cas and gold magnetic nanoparticles, shows great potential as a reliable biosensor for detection of nucleic acid-based targets.

***Keywords:*** Biosensor, Impedance, virus, detection

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**A non-invasive electrochemical genosensensor for detection of C. *difficile***

Hedayatollah Ghourchian

Abstract

Clostridium difficile (C. difficile), is an anaerobic, spore-forming bacterium that causes gastrointestinal infections mainly through the release of two types of toxins (A and B). Usually, in the treatment of microbial infections, one of the most common methods is the prescription of antibiotics. Unfortunately, the arbitrary, incorrect and excessive use of antibiotics has become common in patients. One of the first and most serious problems caused by the excessive use of antibiotics is the destruction of the natural flora of the intestine, which pave the growth and proliferation of opportunistic microbes such as C. difficile, which is transmitted through water and contaminated food in the body. Thus, as a result of the growth and colonization of pathogenic microbes in the intestine, the normal function of this organ is disrupted, and one of the first symptoms of which is diarrhea. This complication is called antibiotic-related diarrhea. Therefore, the measurement of this bacteria at very low levels of concentrations can help the timely treatment of the patient. Recently, in our laboratory, we have developed an electrochemical genosensor, which can detect this bacterium with a detection limit of 0.2 femtomol and a linear response range of 0.5 to 1900 femtomol using differential pulse voltammetry. In this review, this gene sensor is compared with other electrochemical biosensors reported in the literature and its advantages and limitations are evaluated.

***Keywords:*** Clostridioidesdifficile, Electrochemical genosensor, Hexaferrocenium cation, Reduced graphene oxide, Surface layer protein

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**The volatile constituents of rose, saffron and cardamom suppress the fibrillation of tau and not HEWL through the formation of non-toxic tau oligomers**

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**Abstract**

The formation of fibrillar structures of tau is correlated with taupathies including Alzheimer’s disease (AD). This study has aimed to find ways to prevent tau fibril formation. Here, we used dietary compounds including cinnamon (CN), damask rose (Rose), saffron (Saf) and green cardamom (Car), to evaluate the effects of their volatile constituents, on hen egg white lysozyme (HEWL), as a model protein (commonly used for fibrillation studies), as well as the brain-related tau protein. The study was done using different spectroscopic techniques as well as SDSPAGE, AFM and MTT assay. While the results suggested that the volatile constituents were unable to prevent HEWL fibril formation, most of the dietary compounds, in particular Saf, Rose and Car, were able to interfere with the mature fibril formation, by either maintaining the native form of tau or resulting in the entrapment of non-toxic oligomeric forms of tau. Moreover, the neurotoxicity analysis of tau samples on neuroblastoma SHSY5Y cells indicated that tau treated with Saf, Rose and Car were the least toxic. Overall, the findings indicate that the potential therapeutic impacts of the volatile constituents of Rose, Car and in particular Saf, may demonstrate significant efficacy in addressing neurodegenerative diseases such as AD.

***Keywords:*** Natural dietary compounds, Volatile constituents, Tau protein, Fibrillation, Alzheimer’s disease, HEWL

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**Bioremediation potential of Actinomycetes isolated from rhizosphere soil of Lut desert**

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**Abstract**

Bioremediation by microorganisms is a safe method to remove industrial pollutants from soils. Due to special atmospheric conditions, including extreme changes in temperature, salinity, and alkaline pH, desert soil is a suitable substrate for the discovery of bacteria with useful secondary metabolites. According to studies, laccase enzymes derived from bacteria have a high efficiency in breaking down phenolic compounds. Also, some regenerative and antioxidant mechanisms are capable of degrade chemical toxins. In this study, 21 soil samples were collected from five districts of Dehbakari, Rayn, Mahan, Bardsir, and Serbijan in Lut Desert, from the rhizosphere of two plants, camelthorns (*Alhagi persarum*) and globe thistles(*Genus echinops*). Powdery colonies from rhizosphere soil samples were isolated on water agar, and after cultivation in ISP2 specific medium, their cell wall structure (Gram staining), salinity resistance (NaCl 10%), production of laccase enzyme, catalase enzyme, antioxidant properties, and siderophore production were investigated. All 420 isolates were Gram-positive, exhibiting filamentous vegetative mycelia in various colors from white to purple. Results indicate that 52% are catalase producers, 4% are salt-resistant, 31% produce laccase, and 96% generate siderophores. Investigation of the antioxidant properties of Actinomycete isolates is ongoing. According to the results isolated bacteria have biological components necessary for bioremediation activities and decomposition of organophosphorus pesticides. These chemical agents enter agricultural soils as insecticides and cause environmental pollution. The investigation of the effect of selected bacteria on reducing the residues of these chemicals in the soil continues.

***Keywords:*** Rhizosphere, Lut desert, Actinomycetes, Enzyme, Bioremediation

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**Protease enzyme applications and ways to improve its performance**

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**Abstract**

Protease enzymes can hydrolyze peptide bonds. Proteases are widely used in commercial, medical and research processes. Proteases make up 60% of the total market of industrial enzymes. Several proteases of animal origin, such as pepsin, trypsin and proteases of plant origin, such as papain, were discovered and characterized in the early 1800s or the early 1900s, and later microbial proteases were also considered and due to several advantages associated with them quickly became popular. Increasing protease efficiency is critical for various applications, including industrial processes, food production, and biomedicine. Recent research has focused on several strategies to optimize protease performance, including immobilization techniques, engineering methods, and cold-adapted enzymes. The emergence of immobilized enzymes has been a fascinating topic since the 1960s. The idea of immobilizing enzymes was proposed by Nelson and Griffin in 1916 after they found that invertase could hydrolyze sucrose after adsorption on charcoal. Since then, several reversible and irreversible enzyme immobilization methods have been introduced that can enhance the physicochemical properties of enzymes and enable them for practical use.

***Keywords:*** Protease, Enzyme immobilization, Protease application, Cold-resistant protease

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**Theoretical and experimental study of anticancer properties of carboxamide ligand**

Aria Tajally\*, Ahmad Amiri\*, Sudabeh Shokrolahi

**Abstract**

Tetrahydrobenzo [d]thiazole-2,6-diyl) dipicolinamide [H2BPT] which was inspired by biological systems synthesized using green chemistry methods in an ionic liquid solvent. The chemical structure of this compound was confirmed using techniques such as 1H-NMR, IR, UV-Vis, and X-Ray. The interaction of this compound with ct-DNA and human serum albumin (HSA) was studied through fluorescence spectroscopy, CD, and UV-Vis. The results indicated that the binding of the compound to the protein was static and led to a reduction in the alpha-helix structure in albumin. Additionally, at low concentrations, it caused DNA structural distortion, indicating therapeutic efficacy at lower doses. Molecular docking simulations and ADMET studies further confirmed and analyzed the interaction between the compound and biological macromolecules.

***Keywords:*** Carboxamide, Human serum albumin, DNA, Molecular docking, Density functional theory, ADMET

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[**Biophysics of light-sensing proteins and their applications**](https://books.google.com/books?hl=en&lr=&id=5M3WCQAAQBAJ&oi=fnd&pg=PR5&dq=light+sensing+proteins&ots=Cqb14zXwgp&sig=Qu1zgx9QSCQ8kQcykbOEyH_QifE) **in Optogenetics**

Hoda Keshmiri Neghab

**Abstract**

Rhodopsins are photoreceptive proteins and key tools in optogenetics. Although rhodopsin was originally named as a red-colored pigment for vision, the modern meaning of rhodopsin encompasses photoactive proteins containing a retinal chromophore in animals and microbes. Animal and microbial rhodopsins respectively possess 11-*cis* and all-*trans* retinal, respectively. As cofactors bound with their animal and microbial rhodopsin (seven transmembrane α-helices) environments, 11-*cis* and all-*trans* retinal undergo photoisomerization into all-*trans* and 13-*cis* retinal forms as part of their functional cycle. While animal rhodopsins are G protein coupled receptors, the function of microbial rhodopsins is highly divergent. Many of the microbial rhodopsins are able to transport ions in a passive or an active manner. These light-gated channels or light-driven pumps represent the main tools for respectively effecting neural excitation and silencing in the emerging field of optogenetics. A wide variety of light-sensing proteins that are found in plants and microorganisms and that provide natural resources for engineering optogenetic tools are briefly reviewed. We include microbial rhodopsins, which absorb blue/green light; phytochromes, which absorb red/far-red light; UV-A/blue-absorbing flavoproteins (cryptochromes, Light-oxygen-voltage-sensing domain (LOV domain) proteins, Blue Light Using Flavin (BLUF) domain; and the recently discovered UV-B sensor UV RESISTANCE LOCUS8 (UVR8). Among them, the significance of channelrhodopsins, photoactivated adenylyl cyclases, biophysics of rhodopsins and their relationship to optogenetics are reviewed.

***Keywords:*** Optogenetics, Photoreceptor, Light sensing protein

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**Research on a Schiff-base ligand’s interaction with human serum albumin using voltammetry, spectroscopy, and docking**

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**Abstract**

Abstract Human serum albumin, the most abundant plasma carrier protein, has long been the center of attention of pharmaceutical industry due to its ability to bind a diverse range of metabolites and drugs. This astonishing binding capacity often seriously impacts pharmacokinetic properties of drugs. In this work new Schiff-base ligand, 1,1'-((1E,1'E)- (naphthalene-1,5- diylbis(azanylylidene)) bis (methanylylidene)) bis (naphthalen-2-ol) (SNL), was synthesized and the interaction between this ligand and human serum albumin (HSA) was investigated by fluorescence and absorption spectroscopies. A marked decrease in the fluorescence intensity of this compound was observed at 475 nm upon addition of HSA when excitation wavelength was set at 370 nm in pH 7.4 Tris–HCl buffer solution. Reversely, the intrinsic fluorescence of HSA could be quenched by Schiff-base ligand. The quenching mechanism was suggested as static quenching according to the Stern–Volmer equation and the UV–vis absorption spectral change upon addition of HSA. The binding constants Kb and the number of binding sites (n=1) were calculated. Molecular docking results revealed that the primary HSA-SNL binding sites are in the subdomain IA of the HSA structure.

***Keywords:*** Schiff-base, Human serum albumin, Anticancer potential, Molecular properties, Molecular docking

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**Microfluidic device development to study electric field effect on planar lipid bilayers**

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**Abstract**

Various membrane models replicate essential features of biological membranes, including elasticity and fluidity. Planar bilayers have been created using traditional methods, such as the black lipid membrane technique. Recently, micro-fabricated devices featuring horizontally oriented planar lipid bilayers have been developed with combined optical and electrical outputs. Electric fields play important roles in various biological processes, including embryonic development, wound healing, and cancer metastasis. Disruption of epithelial layers can generate lateral electric fields that promote electrotaxis, aiding in tissue repair. Strong electric pulses can induce electroporation, creating temporary membrane pores that facilitate drug delivery. In this study, we designed a microfluidic device using PDMS polymer. We optimized both the bilayer reconstitution method and the aperture design. The optimized 3D–microchip consists of a bottom channel connected to a micromachined upper cone. The capacitance of the bilayer(350 µm diameter) was found to be 500 pF by measuring the impedance. The nonlinear response of the system impedance was studied for different frequencies (100-500 kHz) of the applied voltages. Furthermore, we observed that the membrane's lifespan with a composition of DOPC/DOPS/DOPE (60:10:30) is influenced by the frequency and intensity of the electric field. The bilayer was destroyed by increasing the applied voltage and reducing frequency.

***Keywords:*** Electric field, Microfluidic device, Planar lipid bilayers, Capacitance

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**Inhibition of ACE2 by Beta-defensin-1: A novel strategy against SARS-CoV-2**

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**Abstract**

Beta-defensin-1, an antimicrobial peptide, is considered to be of great importance in our innate immune response. Being a small molecular peptide, it is a wide-range antimicrobial peptide. Conversely, the angiotensin-converting enzyme 2 (ACE2) is utilized by the SARS-CoV-2 virus as the principal entrance to human cells. Due to the importance of these two molecules in COVID-19, this paper focused on the relationship between beta-defensin-1 and ACE2. This study principally aimed at investigating how beta-defensin-1 interacts with the ACE2 enzyme. We attempted to analyze how this interaction affects the function of ACE2 and how, in turn, it protects the host cells from being infected with SARS-CoV-2. For this reason, first of all, PDB structures of ACE2-RBD were retrieved using code 2AJF as well as the beta-defensin-1 structure with code 1IJV from the RCSB database. Energy interaction and molecular docking between beta-defensin and ACE2 were carried out using computational techniques. After that, the resulting interactions were analyzed with the help of molecular dynamics (MD) simulations in order to examine the stability and more details of the interaction. The results obtained demonstrate that beta-defensin-1 interacts with both active and binding sites of the ACE2 enzyme. This binding may also lead to the inhibition of enzyme function, making the targeting of host cells by the virus impossible. This inhibition takes place because of non-covalent associations like hydrogen bonds and van der Waals interactions. Beta-defensin-1 shows great potent ACE2 enzyme inhibition effects, as revealed in our study. Beta-defensin-1 might be a useful drug for treating COVID-19 by preventing the entry of the virus. These results bring new challenges to peptide-based drugs.

***Keywords:*** Beta-defensin-1, ACE2, SARS-CoV-2, COVID-19, Molecular dynamics, Enzyme inhibition

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**Investigating human serum albumin interaction with H2bpb:** **Spectroscopic analysis and molecular docking approaches**

Dorsa Jamali, Ahmad Amiri\*

**Abstract**

Human Serum Albumin (HSA), as one of the main plasma proteins, is crucial in transporting drugs and biomolecules throughout the body [1]. Its interactions with pharmaceutical compounds, such as carboxamides, can significantly impact the bioavailability and efficacy of these compounds. This study investigates the interaction between HSA and a specific Carboxamide. For this purpose, N, N'-(1,2-phenylene) dipicolinamide (H2bpb), was synthesized via triphenylphosphite (TPP) and tetrabutylammonium bromide (TBAB) and characterized with Fourier-transform infrared (FT-IR) spectroscopy [2]. Spectroscopic techniques, including absorbance titration and Circular Dichroism spectroscopy, were employed to analyze this interaction and determine the binding mechanisms. Using Molecular Docking, the binding site on HSA was identified IIA. The results reveal that the bonding between HSA and the studied Carboxamide is primarily mediated by van der Waals forces and π-π stacking interactions, which lead to slight conformational changes in the protein’s secondary structure. These findings offer valuable information for designing new drugs and optimizing existing ones, ultimately enhancing drug delivery methods mediated by HSA.

***Keywords:*** Human Serum Albumin, Carboxamides, Binding Affinity, Molecular Docking

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**Predicting osteoarthritis (OA) using deep convolutional neural network (DCNN) and transcriptome profile**

Moslem Momen

**Abstract**

Osteoarthritis (OA) is a progressive joint disease characterized by cartilage degradation, bone remodeling, and inflammation, leading to pain and loss of mobility. Accurate prediction and early diagnosis of OA remain critical for effective intervention. Recent advancements in deep learning, particularly Deep Convolutional Neural Networks (DCNNs), have revolutionized the field of medical imaging by enabling precise pattern recognition in complex data such as MRI and X-ray scans. Additionally, transcriptome analysis provides valuable molecular insights into gene expression changes associated with OA progression. In this study, we attempted to predict OA by enriching DCNN-based models with transcriptome data to improve prediction accuracy and diagnosis. We hypothesized that by leveraging both DL techniques and gene expression molecular information, we could offer a comprehensive solution for identifying OA at its early stages and guiding personalized treatment strategies. Our results demonstrate that it is possible to accurately predict OA using gene expression data and deep neural networks, even with a limited sample size.

***Keywords:*** Osteoarthritis, Deep convolutional neural networks, Transcriptome analysis, Prediction accuracy, Personalized treatment strategies

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**The effect of mutations caused by DNA oxidation on binding of mitoxantrone to the G-quadruplex**

Masoud Rahimpor Ghadima, Leila Hassania,\*,Zeinb Hatamib

**Abstract**

G-quadruplexes are unique DNA structures formed by sequences rich in guanine that play a role in regulating gene expression. 8- oxo-dG is the most prevalent oxidized form of the nucleotides that causes G > T transversion. This mutation is involved in the pathogenicity of ROS-related diseases. This research investigates the effect of guanine to thymine mutations on the interaction between the anticancer drug mitoxantrone and the four-stranded DNA structure, known as a G-quadruplex, in the promoter region of the c-Myc gene. Mitoxantrone is a topoisomerase II inhibitor that disrupts DNA replication and repair in cancer cells, thereby hindering cell proliferation. Utilizing absorption and fluorescence spectrometry along with gel electrophoresis, we investigated how G to T mutations on the tetrad planes influence on the binding of mitoxantroneto c-Myc G-quadruplex. The results of native PAGE indicated that the mutations change migration pattern and electrophoretic mobility of the G-quadruplex structure implying conformational change of the structure upon the mutations. The percentage of hypochromicity and Stern-Volmer quenching constant of mitoxantrone changes upon the mutations. In addition, the mutations influence on the stability of the interaction in the presence of urea. In conclusion, our findings reveal that specific mutations in guanine caused by oxidative stress alter interaction between the anticancer drug and non-B DNA G-quadruplex structure. These results provide valuable insights for targeted drug design against G-quadruplexes, with implications for enhancing therapeutic approaches in the oxidative stress condition of the cancer cells.

***Keywords:*** G-quadruplexes, c-Myc, Mitoxantrone, Absorption spectroscopy, Fluorescence spectroscopy, Gel electrophoresis

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**Using HSA interaction to investigate the synthesis, characterization, and anti-cancer properties of a CoIII complex**

Melika Nikseresht, Ahmad Amiri\*

**Abstract**

Schiff bases are promising biologically intriguing substances that have a variety of medicinal applications, such as antibacterial, anti-inflammatory, and antipyretic effects. FT-IR, UV-Vis, and elemental analysis are among the spectroscopic methods which are used in this study to synthesize and analyze the [Co (III)(H2L) (1-MeIm)2] Clo4 Schiff base complex. One of our Schiff-bases molecules was found to attach to human serum albumin (HSA) via fluorescence quenching experiments. The binding affinity of the matching complex to HSA has been examined using fluorescence titration studies. It was determined that the computed Kq values were 8.2×1011. Worth noting that these compounds' Kq values are higher than 2.0×1010 M−1s−1. We can infer that static quenching is the main reason of the fluorescence quenching for these Schiff bases. Additionally, we may utilize Scatchard's equation to get the number of binding sites and the binding constant for static quenching. The in- vitro cytotoxicity of the metal complex on the SW-480 cancer cell line was evaluated using the MTT test. The complex exhibited more activity against SW-480 than fluorouracil (FU), with an IC50 value of 0.006μM.

***Keywords:*** Schiff Base, HSA, Anticancer, Fluorescence

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**Optimization of Bioactive Peptide Production from Soy Protein Using Recombinant Protease For Functional Properties**

Yasaman Zandieha, Kimia Aliverdi-Nasabb, Elahe Motamedic, Marzieh Ghollasia,\*, Shohreh Ariaeenejadd,\*

**Abstract**

Plant-derived proteins and peptides have garnered significant interest owing to their versatile functional properties, which go beyond their basic nutritional value. The enzymatic hydrolysis of plant proteins is a controlled and cost-effective method for enhancing these properties. Additionally, the enzymatic breakdown of indigestible carbohydrate components in feed improves digestibility and bioavailability. In this study, soybeans were defatted with n-hexane and subsequently processed using an alkaline extraction method to isolate soy proteins. The protein concentration was quantified using the Bradford assay. The extracted protein was subjected to enzymatic hydrolysis using varying concentrations of recombinant protease to produce bioactive peptides. The degree of hydrolysis was measured and the antioxidant properties of the peptides were assessed using 2,2'-azino-bis3-ethylbenzothiazoline-6-sulfonic acid (ABTS) radical scavenging and reducing power assays. The results demonstrated a significant increase in antioxidant activity, with up to 74% ABTS radical scavenging activity and a reducing power value of 0.347 at 700 nm. These findings suggest that soy-derived proteins and peptides have the potential to enhance the functional properties of both human and animal feeds. These bioactive components can potentially contribute to the nutritional value and functional performance of both human and animal feeds by improving the bioavailability of essential nutrients, offering protective effects against oxidative stress, and enhancing the overall health and growth performance of livestock.

***Keywords:*** Recombinant protease, Soy protein, Bioactive peptides, Antioxidant activity, Reducing power, Enzymatic hydrolysis

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**Interaction Studies of Copper (II) Schiff-Base Complex with Human Serum Albumin and anti-cancer properties**

Samaneh Ghofrani, Ahmad Amiri\*

**Abstract**

The investigation of interactions between drugs and plasma proteins has become a compelling area of research in the fields of chemical biology and pharmacology. Metal-based pharmaceuticals present potential advantages over their organic counterparts, exhibiting modified pharmacological and toxicological properties. A binuclear Schiff base copper (II) complex, [Cu2(HL)2(μ-Br)2]. (H2O), with HL1 being the tridentate ligand 2-(((1-hydroxy-2-methylpropan-2-yl) imino) methyl-4-nitrophenol, was synthesized and characterized utilizing various spectroscopic techniques. Interaction between human serum albumin and the copper (II) complex was investigated by Circular Dichroism and Molecular Docking. MTT assay results indicated that the copper complex demonstrates significant cytotoxicity. These findings suggest that the synthesized complex exhibits promising anticancer properties.

***Keywords:*** Molecular docking, MTT assay, Copper complex, Circular dichroism

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**Synthesis and Identification of CoIII Complex and Protein Binding by Fluorescence and CD Spectroscopy**

Parisa Rezvaninia, Ahmad Amiri\*

**Abstract**

Schiff bases are biologically significant compounds with various medicinal applications, including antibacterial, anti-inflammatory, and antipyretic properties [1,2]. In this study, FT-IR spectroscopy is utilized to synthesize and analyze the [CoIII(H2L) (morpholine)2] ClO4 Schiff base complex. The binding affinity of this complex to human serum albumin (HSA) was assessed through fluorescence titration studies, revealing a calculated Kq value of 6.1 × 10 11. One of our Schiff base molecules was shown to bind to HSA, as demonstrated by fluorescence quenching and CD spectroscopy were employed to analyze this interaction and determine the binding mechanisms. Since the Kq values for these compounds exceed 2.0 × 10 10 M−1s−1 [3], we can conclude that the observed fluorescence quenching in these Schiff bases is due to static quenching.

***Keywords:*** Cobalt Complex, Schiff Base, HSA, anticancer, interaction, CD

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**Interaction of a new Schiff Base ligand with Human serum albumin:** **Insights from spectroscopy and molecular Modeling**

Farzad hosseinia, Ahmad Amirib\*

**Abstract**

Research on the supramolecular interactions between drugs or organic compounds and biological macromolecules has greatly enhanced our understanding of the structures and functions of these bio-macromolecules and various biophysical processes. Human serum albumin (HSA) plays a crucial role in this context, as it binds to most drugs, allowing them to circulate in plasma and reach target tissues. HSA primarily regulates the distribution of these drugs. Consequently, drug-protein binding is a key factor in pharmacokinetics, influencing the drug’s in vivo half-life, unbound concentration, distribution, and elimination. HSA, the most abundant protein in human blood plasma, has a high affinity for numerous endogenous and exogenous compounds, acting as a solubilizer and transporter for drugs and other organic molecules to their intended targets. In this study a new Schiff base ligand (H2L), has been synthesized and characterized by UV–Vis and FT-IR. The interaction between this ligand and HSA was studied through fluorescence spectroscopy and circular dichroism. The intrinsic fluorescence of HSA was quenched by the ligand, which was rationalized in terms of the static quenching mechanism. The results show that this compound can obviously bind to HSA molecules. According to fluorescence quenching calculations, the bimolecular quenching constant (Kq), and apparent quenching constant (KSV) at 27 °C were obtained. The binding constant, Kb, is 110.69 L.mol−1 and the number of binding sites (n) is 1. Furthermore, the CD spectra show that the random coil and antiparallel parts of the secondary structure have trends inverse to the helix part in the presence of Schiff base ligand.

***Keywords:*** Schiff base, Human serum albumin, Anticancer potential, Molecular properties, Molecular docking

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**The effect of guanine oxidation on the interaction of the doxorubicin whit four-stranded DNA**

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**Abstract**

Four-stranded structure are guanine-rich sequences that are involved in the expression of proto-oncogene such as c-Myc.Doxorubicin is an anticancer drug belonging to the anthracycline family, which exerts its biological effect by inhibiting the topoisomerase II enzyme, chromatin instability and DNA breaks. In this research, the effect of guanine oxidation on the interaction of doxorubicin with the four-stranded structure of the NHE III region of the c-Myc gene promoter has been investigated. Absorption spectroscopy, Fluorescence emission and polyacrylamide gel electrophoresis were used to evaluate the interaction. The results of spectroscopy showed that the oxidation of guanine in the tetrad plane of the four-stranded structure causes a change in the binding of doxorubicin.The results of absorption spectroscopy indicated that percentage of the drug hypochromicity decreases upon addition of the oxidized G-quadruplex DNA structure in compared with the wild type structure. Fluorescence spectra implied that emission of doxorubicin decreases upon interaction of the both forms of G-quadruplex DNA, but the oxidation of guanine in the tetrad plane causes a remarkable decrease in the DNA concentration where binding saturation occurs. The binding constant of the G-quadrulex to doxorubicin and Stern-Volmer quenching constant decrease due to oxidation of the guanine nucleotide. In addition, the oxidation influences on stability of the interaction in the presence of urea and the electrophoretic mobility of the DNA structure in native polyacrylamide gel. Consequently, our results imply that oxidative stress can mediate cancer initiation and development by molecular damage of the nucleotides have remarkable effect on the interaction between doxorubicin anticancer drug and the G-quadruplex non-B DNA structure.

***Keywords:*** Four-stranded structure, Doxorubicin, Guanine oxidation, c-Myc gene

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**A study on the interaction between human serum albumin (HSA) and Fibroblast activation protein inhibitor (FAPi): Experimental and theoretical perspectives**

Sudabeh Shokrollahia, Ahmad Amirib,\*

**Abstract**

Fibroblast activation protein (FAP) is a membrane-bound protease that has limited expression in normal adult tissues but is highly expressed in the tumor microenvironment of many solid cancers. Among them, a class of FAP inhibitors (FAPi) with a N-(4-quinolinoyl)-Gly-(2-cyanopyrrolidine) scaffold displayed nanomolar affinity and high selectivity against other interfering dipeptidyl peptidases and prolyl oligopeptidase. FAP-2286 is a FAP-binding peptide coupled to a radionuclide chelator that is currently being investigated in patients as an imaging and therapeutic agent. FAPI-46 is a quinoline-based fibroblast activation protein (FAP)-targeted radiotracer. FAPI-46 has higher tumor uptake and prolonged tumor accumulation. FAPI-46 can be used for tumor imaging of a multitude of different cancers 1-2]. In this study, FAPi-46 and FAP-2286, as well-known FAP inhibitor, were selected and prepared. Furthermore, the binding affinity between the above-mentioned inhibitors and human serum albumin (HSA) were studied under simulated physiological conditions (using molecular docking (MD)) and experimental analyses (using fluorescence and CD spectroscopies and cyclic voltammetry). The obtained results revealed that the formation of a complex between HSA and drugs were responsible for quenching the native fluorescence of protein at 343 nm and can be illustrated by the static mechanism. The binding constant and number of binding sites were considered and proposed that the combination of hydrophobic and electrostatic forces were the principal intermolecular forces stabilizing the complex. Also, theoretical results show that the both of drugs have high affinity for binding to HSA.

***Keywords:*** FAP, Human serum albumin, anticancer potential, Molecular properties, Molecular docking

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**Encapsulation of phytase using freeze-drying method to enhance performance and stability**

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**Abstract**

Phytase is a critical enzyme in the feed industry for livestock, poultry, and aquaculture, as it facilitates phosphorus absorption and improves the digestibility of other nutrients. Given its essential role, extensive research has been conducted on encapsulation techniques to preserve and stabilize phytase activity under harsh environmental and gastrointestinal conditions. We investigated a novel phytase enzyme that demonstrates optimal activity for reducing phosphorus-related pollution. By analyzing soil samples with an enhanced selective culture medium, we successfully isolated bacterial phytase producers. We extracted enzymes from these bacterial isolates and measured their phytase activity. Our characterization of the phytase included optimal pH, temperature, and substrate specificity. In the current study, we used chitosan, gum Arabic, and gelatin as encapsulation materials. Freeze-drying, a widely recognized and industrially practical method, was employed to dry the encapsulated enzyme samples. This encapsulation strategy aims to enhance the enzyme's resistance to temperature and pH fluctuations, ensuring its functionality throughout the storage and digestive processes. To confirm the encapsulation of phytase, the enzyme was labeled with fluorescein isothiocyanate (FITC), and fluorescence microscopy images validated the successful encapsulation. The encapsulated phytase demonstrated superior activity and stability compared to the free enzyme, showing better performance in terms of enzyme activity retention and prolonged shelf life. The results of this study have significant implications for the development of more efficient and stable phytase supplements, potentially enhancing nutrient absorption and reducing environmental phosphorus pollution from animal waste.

***Keywords:*** Enzyme Encapsulation, Freeze-drying, fluorescein isothiocyanate, enhancing nutrient absorption and environmental phosphorus pollution, Phytase

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**From functionalization to characterization: Investigating tryptophan-functionalized carbon nanotubes and unveiling its properties**

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**Abstract**

Nanobiotechnology is a combination of nanotechnology and biotechnology that suggests new methods to produce lighter and stronger materials widely used in biology and medicine. Carbon-based nanomaterials are one of the tools of nanobiotechnology, and we can mention carbon nanotubes (CNTs) as one of the most important of them. They are classified into multi-walled (MWCNTs) and single-walled (SWCNTs) CNTs categories. As CNTs are insoluble in water and are toxic for cells, we can functionalize them with various agents to improve their performance. In this study we functionalized MWCNTs with tryptophan an essential amino acid with unique properties and potential applications in biomedicine and nanotechnology. Then we use scanning electron microscope (SEM) and FT-IR analyses to ensure in functionalization of MWCNTs. Results from these analyses show that functionalization of MWCNTs have be done correctly. Functionalization of MWCNTs makes lower their insolubility and toxicity and improve their performance in cell environment. Now they can be used in biological and medical applications like drug delivery, biosensing, tissue engineering and so on.

***Keywords:*** Carbon nanotubes, Functionalization, Nanobiotechnology, Multi-walled carbon nanotubes

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**Bioinformatics studies on the F87D mutation in the photoprotein Mnemiopsin 2**

Amir Reza Mohammadi\*, Fatemeh Khatami, Vahab Jafaria

**Abstract**

Calcium-regulated photoproteins are a type of non-enzymatic proteins capable of emitting light, with a wide range of applications in biological and agricultural studies. Mnemiopsin 2, a member of this group, consists of two primary parts: an apoprotein (apomnemiopsin) and a chromophore containing coelenterazine and oxygen, bound non-covalently. These photoproteins are extensively utilized in fields such as protein-protein interactions, calcium signal tracking, gene expression analysis, and drug discovery. Mnemiopsin 2 contains three active EF-hand motifs (I, III, and IV), which can bind calcium ions, while EF-hand II cannot. Each EF-hand has a conserved helix-loop-helix structure essential for calcium binding. This study employs bioinformatics tools and physico-chemical measurements to analyze the structural and functional changes in Mnemiopsin2 mutated at position 87, comparing it with the wild-type protein. Using Medeller (v10.4) and Chimera (v1.13.1) software, along with parameters like RMSD, ERRAT, and Ramachandran score, we identified the most optimal model. Additional analysis, including hydrophobicity and accessible surface calculations, were conducted using resources like ProtParam, VADAR, and Protscale on Expasy. This comprehensive analysis offers insights into the potential applications of mutated Mnemiopsin 2 in biological fields. It was found in this instance that the protein's hydrophobicity was not significantly changed by the F87D mutation. Furthermore, the instability was furthered by the F87D mutation. The mutation did not lead to any remarkable alterations in the protein's structure when compared to the wild-type protein.

***Keywords:*** Bioinformatics, EF-hand, Mnemiopsin2, Molecular modeling, Photoprotein

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**Investigation of Glycine 96 roles in EF-handII photoprotein Mnemiopsin 2: Bioinformatics Studies**

Zahra karimia,\*, vahab jafarianb, Amir Dehghania

**Abstract**

Bioluminescence is the process of light emission by some living organisms. Mnemiopsin 2, a Ca2+ regulated photoprotein isolated from *Mnemiopsis leidyi*, having a blue ﬂash type emission and belongs to family of ctenophore photoproteins. Photoprotein mnemiopsin 2 is a single subunit protein consisting of 207 amino acid residues. These photoproteins have been exploited as markers or reporters for biochemical processes in biological and biomedical researches. They are precharged bioluminescent proteins that are triggered to emit light by binding Ca2+ or certain other inorganic ions. They contain three EF-hand domains to bind Ca2+, and accommodate a peroxidized coelenterazine in the central cavity of the protein. Ctenophore photoproteins also contain three canonical sequence loop regions, each of 12 contiguous residues, which supply the oxygen ligands needed for calcium ion coordination. The residue of Glycin 96 is the twelfth residue in the EF-hand II loop of mnemiopsin 2, EF-hand II has lost its function during evolutionary stages. For this purpose, Glycin 96 was replaced with Glutamate residue (G96E). The three-dimensional structure of mutant was made with MODELLER program V. 10.4 and the best structure was evaluated using ModEval, SAVES. VADAR and ProtParam servers were used to calculate the interactions, Structural stability and physico-chemical properties of protein. ProtScale server showed Kyte & Doolittle hydropathy plot.Then, the graphical form of the desirable model was drawn using the UCSF Chimera software Finally, the optimized models were compared with the native model, The results indicate that the mutated model is slightly unstable than the native model, And it also increases the polarity in its structure. However, the free energy of G96E mutant has increased compared to native, and indicates the sturactural stability of the mutant.

***Keywords:*** Molecular Modeling, Photoprotein, Site-directed mutagenesis, Stability

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**Synthesis, characterization, and drug-Like interaction evaluation of Copper Schiff Base complex with Human Serum Albumin**

Kowsar Zabihpour\*, Ahmad Amiri\*, Sudabeh Shokrolahi

**Abstract**

In this research, a novel Copper Schiff Base Complex was designed and synthesized, evaluated for its unique properties as a drug-like compound. Its molecular structure was confirmed using advanced techniques such as 1H-NMR, IR, UV-Vis, and X-Ray, which collectively verified the integrity and accuracy of the molecular configuration. Understanding the interaction of potential drug candidates with target proteins in the body is critical in pharmaceutical development. Therefore, we focused on assessing the interaction of this complex with human serum albumin (HSA) using fluorescence spectroscopy and circular dichroism (CD) techniques. The results revealed a specific interaction between the complex and HSA, highlighting its potential therapeutic efficacy and safety profile. Furthermore, to gain deeper insights into the type and mechanism of molecular interactions, molecular docking simulations were employed. These simulations provided valuable information regarding the binding sites and interaction mechanisms of the complex with biological machinery, paving the way for further development of this complex as a potential therapeutic agent.

***Keywords:*** Copper Schiff Base Complex, Human serum albumin, Molecular docking circular dichroism, Fluorescence spectroscopy

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**Characterization of gold nanoparticles conjugation to oligonucleotides as a nanoprobe in a cancer diagnostic biosensor**

Negin Saatia, Hamidreza Mollasalehib,\*

**Abstract**

Biosensors are widely used in point-of-care tests for quick, easy and non-invasive measurements. The diagnostic sensitivity of the biosensor is increased by using gold nanoparticles and their optoelectronic properties. The purpose of this study is to investigate the binding of nanoparticles to the selected sequence of oligonucleotides, in order to be used in cancer diagnostic biosensor. In that regard, the oligonucleotide sequence was selected and the nanoprobe was designed. Afterward, functionalization of gold nanoparticle was performed using a type of phosphine as an ionic reducer after multiple incubations in 72 h. Thus, after nanoprobe production, salt tolerance (nanoparticle stability), FTIR, zeta potential and DLS tests were performed to analyze the nanoparticle conjugation to the selected sequence. In the stability test, the nanoparticles are precipitated in the vicinity of a high concentration of salt and the solution turned gray. In contrast, the nanoprobe retained the initial red color. A spectroscopic analysis at 300-800 nm showed that the nanoprobes had an absorption peak in the red wavelength range (around 500 nm), while the nanoparticles had no peak in this range. In the Fourier-transform infrared spectroscopy method, a peak was revealed in the wavelength range of 950 to 1050 indicating the sugar phosphate band in the nanoprobe. DLS results showed that after functionalization, the size and distance between nanoparticles increased from about 30 nm. Furthermore, in the zeta potential test, the charge of nanoparticles decreased to -10 mV, which can indicate the successful functionalization and production of nanoprobes for the purpose of cancer diagnosis. This study could revolutionize the design of simple and fast diagnostic biosensors for cancer detection with extremely sensitive and selective power in biological molecules.

***Keywords:*** miRNA, AuNPs, Characterization, FTIR, Zeta potential, DLS

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**Effects of organic solvent and ionic liquids on the kinetic behavior of chromate reductase**

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**Abstract**

Organic solvent and ionic liquids (ILs) have received increasing attention as attractive solvents in medical and biotechnological usages. The present study has been carried out to study the comparative influence of 1-butyl-3-methylimidazolium, 1-methylimidazolium and some organic solvent on the kinetic parameters of the chromate reductase. Km and Vmax values for enzyme were calculated 1.39 mM and 0.26 μ mol.min-1.mg-1, respectively. As the concentration of ionic liquids increased, Km increased and kcat decreased. In addition, the associated tertiary structures changes of enzyme caused by ILs (100 mM) were studied by fluorescence method. The enzyme activity in the presence of 0.5 mM [MIm][Cl] and 0.4 mM [MIm][BF4] reduced to 35% of the initial reaction rate whereas this enzyme demonstrated 76% of its initial activity in the presence of organic solvent such as Tween 20, indicating that the chromate reductase is more sensitive to these ILs compared to Tween 20.

***Keywords:*** Organic solvent, Ionic liquids, Chromate reductase

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**Effect of charge change on the EF-hand II recovery in Mnemiopsin 2 by H95D mutation**

Hanieh Ramezany\*, Fatemeh Khatami, Vahab Jafarian

**Abstract**

Bioluminescence is the phenomenon of visible light emission by living organisms which chemical energy is converted into light energy. This globular photoprotein consists of 207 amino acids with a molecular weight of 24 KD. This photoproteins has 4 EF-hand with a helix-loop-helix structure that are Ca2+ binding sites. 3 residues, aspartic acid, at position 1; glycine, at position 6, and glutamic acid, at position 12, are conserved. It is worth mentioning that EF-hand Ⅱ has lost this ability. Also, Mn2 has a hydrophobic cavity that forms coelenterazine binding site. The aim of this work is to investigate the structural and functional properties of the mutated protein H95D in order to recovery the EF-hand Ⅱ activity. Thus, at first Mnemiopsin 2 amino acid sequence was obtained from the NCBI database and mutant models were designed. Finally, the sequence alignment of the wild-type protein along with the mutant protein, aequorin, obelin, and berovin was aligned with Clustal W and checked by through the ESPript3 server. Using Modeller version 9.20, three-dimensional structures of both wild-type and mutated protein were generated. Using VADAR, SAVES and ModEval servers, the best model was confirmed based on the parameters such as WHATCHECK, PROCHECK, z-DOP, ERRAT and RMSD. The ProtScale server was used to drawing hydropathy plots, while several biochemical parameters were calculated by using ProtParam. The results show that this mutation caused increased the structural stability of the protein.

***Keywords:*** EF-Hand, Molecular modeling, Photoprotein, Site-directed mutation

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**Molecular docking of BACE1 enzyme with ferulic acid and p-coumaric acid in Alzheimer's disease**

Tooba Abdizadeh

**Abstract**

Alzheimer's disease (AD) is a brain disorder that affecting a large population worldwide is characterized. This disease has no definitive treatment and imposes a great economic burden on the patients' families, and therefore, improvement of treatment methods is needed. β-site amyloid precursor protein-cleaving enzyme 1 (BACE1) acts as a rate-limiting step in the production of amyloid beta (Aβ) that alters the course of Alzheimer's disease. Abnormal activity of BACE1 in the brains of people with AD leads to the formation of beta-amyloid proteins. Receptor-ligand binding studies were performed using Autodock software. The ligands of ferulic acid, p-coumaric acid, and donepezil, were taken from Pubchem and converted into PDB format by AutoDock software for docking analysis. Afterward, the BACE1 protein was received from the Protein Data Bank, and after the preparation of this protein, molecular docking was done with these ligands by using the Autodock software. Finally, the obtained results were analyzed. Molecular docking shown high binding affinity for selective ligands to BACE1 enzyme. The ligands interacted with residues Asp228, Lys224, and Asp32 of BACE1, all of which fall within the active site of the enzyme, which may be critical for BACE1 inhibitory activity. This study provided evidence to consider these ligands as a valuable small molecule in the treatment and prevention of AD-related diseases, and further research in- vitro and in vivo may show their therapeutic potential.

***Keywords:*** Alzheimer's disease, Ferulic acid, p-Coumaric acid, Molecular docking

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**Evaluation of folate-conjugated green synthetized gold nanoparticle potential for human colorectal adenocarcinoma and gastric cancer therapy**

Nasrin Mollaniaa,Fariba Mollaniab, Fateme Malayjerdia, Fateme Zahra Bagheri-Nezhada, Hanieh Nozhatia

**Abstract**

One of the important applications of green biosynthesized gold nanoparticles by medical plants is their use as a carrier in drug delivery for cancerous cell treatment. In cancer, a group of body cells undergoes irregular proliferation that can subsequently invade other tissues and adjacent organs and ultimately cause metastasis and spread throughout the body. Many anticancer drugs need to be released at the appropriate concentration and in a suitable place to have the best effect; hence, this work has tried to develop beneficial nanomaterials by medicinal plants such as *Salvia rosmarinus* extract in the biomedical field. This work considered the development of a new biological system with the least side effects and the most impact, and the gold nanoparticles as carriers were biosynthesized. On the other hand, for more impact, the non-covalent nanoparticle and folate interaction was done. Human Colorectal Adenocarcinoma and gastric cancer are two foremost among many carcinoma cases globally and most of the enhanced treatments could not significantly decrease the mortality range of these cancers. The current work is planned to develop a folate-conjugated green synthesized gold nanoparticle that are effective drug against these diseases. Therefore, for the cytotoxicity assay by MTT assay, the HT-29 and gastric carcinoma (AGS) cell lines were selected, respectively. In the results, the nanoparticles in the presence of folic acid have the best effect on these cancer treatments.

***Keywords:*** Green synthetized nanoparticle, Gold nanoparticle, Cancer therapy, Colorectal and gastric cancer

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**Kinetics of Caspase7 thermal inactivation**

Fatemeh Zaare\*, Jamshid Davoodi

**Abstract**

Caspase 7 is a cysteine protease that induces programmed cell death in the internal pathway of apoptosis. The active enzyme consists of a homodimer of a hetero dimer. Thus, we sought to determine the mechanism of inactivation, i.e. aggregation versus the loss of the qurternary structure. For this purposee, recombinant caspase7 protein was expressed and purified by affinity chromatography method. The purified enzyme was subjected to elevated temperatures for a period of 0 to 16 hours. Then the enzymatic activities of aliquates withdrawn at certin time points were measure by the hdrolysis of the chromogenic substrate DEVD-pNA monitored at 405 nm. The enzyme was completely inactive following 10 hours incubation at 37 degrees. SDS-PAGE analysis of the samples revealed no hydrolysis of the proteins due to self celavage or by proteases that migh be presnt as minor impurities. Analysis of the kinetics of enzyme inactivation by fitting to 1st and 2st degree equations showed that that enzyme inactivation follows the 1st degree equation. This indicates that either the hetero dimer is being dissociated or homodimer is falling apart leading to loss of activity.

***Keywords:*** Caspase7, Inactivation, Denaturation

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***In-silico evaluation of anti-cancer ligands targeting the leucine-rich repeat-containing G protein-coupled receptor 4***

Soodabeh Shafiee

**Abstract**

Leucine-rich repeat-containing G protein-coupled receptor 4 (LGR4/GPR48) has recently emerged as a critical player in various malignancies, including breast cancer, participating in tumor progression, invasion, and metastasis. LGR4 inhibitors are currently being explored for a variety of medical applications, with cancer therapy being the most promising application. The extracellular domain of LGR4 (LGR4-ECD) has shown potential as a new therapeutic for cancer. In this study, a molecular docking-based screening approach was used to identify the natural compounds with anti-breast cancer activities. The 3D structure of LGR4 protein (PDB ID: 4QXE) was retrieved from PDB, RCSB. Several natural compounds including Myricetin, Quercetin, Apigenin, Luteolin and Baicalein were chosen to be investigated as LGR4 binders. Ligands were acquired in their 3D conformer forms from the PubChem database. The structures of both the protein and ligands were subsequently prepared for molecular docking using Molegro Virtual Docker (MVD). From protein-ligand interaction analysis and binding energies determined following docking, we found that the Baicalein had the highest binding affinity to the target protein (MolDock Score of −118.95). These findings may provide important information for developing anti-breast cancer therapeutics targeting LGR4.

***Keywords:*** Leucine-rich repeat-containing G protein-coupled receptor 4, Breast cancer, Docking simulations, 3D structure

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**Study of the interaction between Schiff base complex and human serum albumin by fluorescence spectroscopy**

Melika Nikseresht, Ahmad Amiri\*

**Abstract**

New Schiff-base has been synthesized from the 1:1 M condensation of 2,2'-((1E,1'E)-(1,2-phenylenebis (azaneylylidene)) bis(methaneylylidene))bis(4-bromophenol) (H2L) with Co(OAC).4H2O. The present study aims to investigate and identify the modes in the binding of the Schiff base complex to human serum albumin (HAS). Hence, [ Co(H2L)(Py)2]ClO4complexe has been characterized by spectroscopic methods such as infrared and 1H-NMR as well as chemical analysis. Also, the studies on the interactions between metallodrugs and HSA, as carriers for drugs and biological molecules, are extremely important to design new drugs. In this study, the interaction between HSA and newly designed anti-cancer compounds has been investigated. Circular dichroism and fluorescence quenching studies revealed one molecule of our Schiff bases to bind to HSA. The number of binding sites, the Stern-Volmer quenching constant and the association constant of the complex were calculated on the HSA protein. According to the results, these complexes can bind to the main blood carrier protein HSA and change the secondary structure of the protein Schiff base complex is shown. The in- vitro cytotoxicity of the metal complex on the SW-480 cancer cell line was evaluated using the MTT test. The complex exhibited more activity against SW-480 than fluorouracil (FU), with an IC50 value of 0.107μM.

***Keywords:*** HAS, Schiff base, Anti- cancer, Fluorescence

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**Controllable fabrication and characterization of green synthesized ZnO nanoparticles**

Fayezeh Samaria,b,\*, Saeedeh Majnoonpour a

**Abstract**

Zinc oxide nanoparticles (ZnO NPs) are regarded as highly attractive multifunctional nano-semiconductors owing to their exceptional photostability, wide bandgap, non-toxic nature, thermal stability, cost-effectiveness, corrosion resistance, biocompatibility, wide absorption spectrum, and notable antioxidant, antimicrobial, antibacterial, and anticancer properties [1]. Also, the Food and Drug Administration has recognized it as a safe substance for human use [2]. With these regards, the green synthesis of ZnO NPs using plant extracts has driven tremendous interest in recent years [3]. This research aimed to facilitate the phyto-fabrication of ZnO NPs using the aqueous leaf extract of *Manilkara zapota* (*M. zapota,* commonly known as Chikoo) as a renewable and non-toxic reducing agent and effective capping agent in the synthesis process. The study investigated the effects of varying leaf extract quantities and calcination temperatures to determine the optimal conditions for synthesis. The physicochemical characteristics of the synthesized ZnO NPs were evaluated using ultraviolet-visible spectroscopy (UV-Vis), X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM), and energy-dispersive X-ray spectroscopy (EDS). The ZnO NPs derived from the leaf extract of *M. zapota* displayed a broad absorption band in the range of 356–369 nm, indicative of the intrinsic band-gap absorption of ZnO, thereby confirming the formation of ZnO NPs. FE-SEM imaging revealed that the majority of the nanoparticles are spherical, with diameters ranging from 35 to 75 nm. EDX analysis validated the presence of zinc and oxygen, confirming the successful production of ZnO NPs. Finally, the XRD pattern corroborated their crystalline nature with a hexagonal wurtzite structure.

***Keywords:*** Green synthesis, ZnO nanoparticles, *Manilkara zapota* leaf extract, Characterization

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**Bioinformatics analysis of the BRI1-associated receptor kinase (BAK1) in Arabidopsis thaliana and its comparison with Homo sapiens orthologue**

Mehdi Safaeezadeh, Masoumeh Fallah Ziarani

**Abstract**

BAK1 gene plays a role in apoptosis as well as in autoimmune diseases. Due to the importance of this gene, the stability of this gene was investigated in Arabidopsis and humans, and the results showed that this gene is one of the unstable genes in both humans and Arabidopsis.

***Keywords:*** BAK 1, Apoptosis, Arabidopsis, Autoimmunity

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**Nanozyme, a new horizon in artificial enzymes**

Fatemeh Honarasa

**Abstract**

Nanozymes are nanomaterials with intrinsic enzyme-like properties. As an artificial enzyme, nanozymes take advantage of good stability, easy modification, designability, ease of preparation, and low cost. Nanozymes have been booming over the past decade because of their capability to address the limitations of natural enzymes such as low stability, high cost, and difficult storage. Along with the rapid development and ever-deepening understanding of nanoscience and nanotechnology, nanozymes hold promise to serve as direct surrogates of traditional enzymes by mimicking and further engineering the active centers of natural enzymes. In recent years, a great number of nanozymes have been fabricated. Nanozymes were synthesized in different spatial dimensions (0D, 1D, 2D, 3D). Moreover, over the past decade, multi-functional nanozymes have been developed for various applications. The nanozymes were applied for disease diagnosis, tumor microenvironment sensing, pathogen detection, drug detection, food detection, and environmental sensing. In this work, a short review on nanozymes, their mechanism and applications were provided.

***Keywords:*** Nanozyme, Artificial enzyme, Enzyme-mimetic, Catalyst

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**Reltecimod sodium synthesis optimization**

Kaghazian Hoomana,\*, Zarei Zahrab

**Abstract**

Reltecimod sodium acetate is a salt of the synthetic peptide (H-D-Ala-Ser-Pro-Met-Leu-Val-Ala-Tyr-Asp-D-Ala-OH) binds and modulate CD28 co-stimulatory receptor that provides protection from bacterial super antigen toxins and from lethal bacterial infections in experimental models of a wide range of bacterial pathogens (both Gram positive and Gram negative. The sequences were synthesized at room temperature on 2-CTC resin with HATU activation using an orbital shaker. Amide bond formation was performed in 60 minute, and Fmoc group were removed in 30 minute with 25% (v/v) piperidine in DMF, after completion of synthesis, the resin-peptide were washed with DMF (3×), The peptide is separated by performing the following steps: first of all adding dichloromethane and MeOH and then dried by Filtration system, after that we use cleavage solution including: TFA, TES, Me OH, the solution under the filter is separated and most of it is removed by rotary evaporator and the remaining solution is added to the cold diethyl ether and the white precipitate was collected. We did purification by Preparative HPLC (c18 column). The synthesis of the final material was confirmed with high yield by HPLC, mass spectrometry.

***Keywords:*** Optimization, Peptide synthesis, Reltecimod Sodium, Chemical synthesis

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**Investigation of genetic, structural, and physicochemical diversity of Acyl Homoserine Lactones in Bacillus species**

Nasim Forghania, Matia Sadat Borhania,\*, Zhoheir Heshmatipourb, Mahmoud Salehia,\* Mohadeseh Piric

**Abstract**

The quorum sensing (QS) system is a key communication mechanism in microorganisms, playing a role in regulating processes such as biofilm formation. Bacteria communicate via autoinducer molecules, and when the concentration of these molecules reaches a specific threshold, certain genes are activated, causing physiological changes in the microbial community. One of the most important autoinducers is N-acyl homoserine lactone (AHL), which is degraded by lactonase and acylase enzymes, disrupting QS and pathogenicity. Bacillus species are among those that produce AHL-lactonase, which breaks down these molecules. This study aims to investigate the diversity of the gene encoding AHL-lactonase in Bacillus and its impact on the enzyme's structure, physicochemical properties, and interactions with QS ligands. In this research, 130 Bacillus isolates were collected from soil in various regions of Iran. Among the nine isolates containing the gene, isolate ELMX2B was selected for further studies. The genes were amplified via PCR and sequenced, the enzyme's 3D structure was predicted using Swiss-Model, and molecular docking studies were conducted. The results indicated a high similarity in sequences and genetic relatedness of these enzymes to GenBank data, and the ELMX2B lactonase showed the highest binding affinity to C12-HSL (ΔG = -6.7 kcal/mol) compared to the reference lactonase. Additionally, it was found that variations in the ligand's carbon chain length did not affect the enzyme's binding affinity. Physicochemical studies demonstrated that the stability of the target lactonase is higher than that of the reference enzyme.

***Keywords:*** Quorum sensing, Molecular docking, Homology modeling, Acyl-homoserine lactones

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**The impact of diabetic glucose concentration on viability and cardiac differentiation of mesenchymal stem cells**

Shadi Nosratia, Maryam Gheisaria, Shahrokh Zareb, Mahintaj Darab, Samaneh Zolghadric, Iman Razeghian-Jahromid,\*

**Abstract**

~~Introduction:~~ Hyperglycemia may be a stumbling block for delivery of regenerative benefits of mesenchymal stem cells (MSCs) to diabetic patients with cardiovascular diseases. Our study aims to assess the viability and cardiac differentiation potential of MSCs after being exposed to diabetic glucose concentration.

~~Methods~~: MSCs were extracted from rat bone marrow. Cells were characterized based on morphology, differentiation potential, and expression of mesenchymal specific markers. MTT assay was done to evaluate the viability of MSCs after treatment with different glucose concentrations. Case group was MSCs treated with diabetic concentration of glucose versus cells treated with PBS as the control group. Growth curve and population doubling time were calculated in both groups. Expression of GATA4 and troponin, as the early and late markers during cardiac differentiation, were measured following 5-azacytidine exposure.

~~Results~~: Proliferated cells at passage three had fibroblastic-shape, was able to differentiate into adipocytes or osteocytes, and expressed CD73 and CD90. MSCs viability was gradually decreased by increasing glucose concentration. Irrespective of nicotine concentration, three-day exposure imposed more severe detrimental effects on viability compared with one-day treatment. Proliferation rate of the MSCs was lower in the case group, and they need more time for population doubling. Expression of both cardiac markers were downregulated in the case group at day three. However, their expression became higher at day seven.

~~Conclusion~~: Diabetic glucose concentration inhibits normal proliferation and cardiac differentiation of MSCs. This effect should be considered in stem cell therapy of cardiovascular patients who are concurrently affected by hyperglycemia, a common comorbidity in such individuals.

~~Why carry out this study?~~

Stem cell therapy has opened a promising window to reduce great burden imposed by cardiovascular disease.

Despite substantial benefits observed in early studies, clinical translation of such treatment approaches has been hampered.

Hyperglycemic condition may be one of the hurdles responsible for reduced beneficial effects of stem cell therapy in cardiovascular patients.

~~What was learned from the study?~~

Findings of our study revealed that diabetic glucose concentration inhibits normal proliferation and cardiac differentiation of mesenchymal stem cells.

Since diabetes is one of the common comorbidities in patients with cardiovascular diseases, glycemic status of such patients should be considered in the time of stem cell transplantation.

Moreover, these patients may need some pretreatments or augmented cells for transplantation in order to observe maximum benefits.

***Keywords****:* Glucose, Diabetes, cardiovascular disease, Mesenchymal stem cells, Proliferation, Differentiation

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**Investigating the factors influencing human serum albumin fibrillation using thioflavin t**

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**Abstract**

Protein fibrillation, a process implicated in various neurodegenerative diseases, is a critical area of study for understanding amyloid-related pathologies and developing therapeutic strategies. This study utilized human serum albumin (HSA), a well-characterized model protein, to explore how temperature, pH, and protein concentration affect fibrillation. A Central Composite Design (CCD) experimental framework was implemented, assessing three levels for each factor: temperature (37°C, 47°C, and 57°C), pH (3, 5, and 7), and concentration (1, 1.5, and 2 mg/mL). Fibrillation was induced over a 48-hour period at a stirring speed of 300 rpm, with aggregation monitored using thioflavin T (ThT), a fluorescent dye that selectively binds to amyloid fibrils, allowing real-time observation of the fibrillation dynamics. Fluorescence intensity was recorded at an excitation wavelength of 440 nm and emission wavelengths of 450 nm and 600 nm. Results indicated that the combined effects of temperature, pH, and concentration significantly influenced HSA fibrillation, with aggregation observed. The quadratic model accounted for 92% of the variance in yield, highlighting significant contributions from concentration. Normalization was performed using a power transformation of -1.24. The model demonstrated significance with a p-value of 0.0013 and an F-value of 10.85. The optimal conditions identified were a concentration of 2 mg/mL at 57°C and pH 3. This research enhances our understanding of the conditions that facilitate fibrillation.

***Keywords:*** Protein Fibrillation, Human Serum Albumin, Thioflavin T, Amyloid-related diseases

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**A Novel technique for detection of Tryptophan using carbon quantum dots synthesized from plastic waste**

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**Abstract**

Tryptophan, an essential amino acid, plays a unique and critical role in biology due to its distinctive structure and functions. Its indole side chain, featuring an aromatic, binuclear ring, sets it apart among amino acids, and it exists in cells at notably low levels. As humans cannot synthesize tryptophan, it must be obtained from dietary sources. In the body, tryptophan supports protein synthesis, growth, and overall health and acts as a precursor to several important biomolecules, including the neurotransmitter serotonin, the hormone melatonin, and niacin. Deficiencies in tryptophan are linked to a range of metabolic and neurological disorders, underscoring the importance of accurate detection in both food and biological samples. Variations in tryptophan levels are associated with numerous health conditions, including depression, cancer, and cardiovascular disease. For example, reduced tryptophan levels can serve as a biomarker for diabetic nephropathy, colorectal cancer, and Alzheimer’s disease. In the fields of food safety, clinical diagnostics, and biochemical research, monitoring tryptophan and its metabolites is essential to understanding metabolic processes and assessing nutritional quality. Fluorescent nanoparticles, especially carbon quantum dots (CQDs), have garnered significant attention for their applications in bioimaging and sensing. Synthesizing CQDs from plastic waste, such as polyethylene terephthalate (PET), offers an environmentally friendly approach to repurposing waste materials for scientific applications. In this study, CQDs synthesized from PET via a hydrothermal method were used for the detection of tryptophan. The addition of tryptophan effectively quenched the fluorescence of the CQDs, demonstrating a novel approach for tryptophan detection.

***Keywords:*** Tryptophan, Optical sensor, Graphene quantum dots (GQDs), Circular economy, Waste upcycling, Bioimaging

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**Synthesis, characterization and biocompatibility evaluation of bone cement composite reinforced with squid bone (*Sepia Officinalis*)**

Mahdis Ahmadia, Azadeh Hekmata,\*, and Aghdas Banib

**Abstract**

Calcium phosphate ceramics have limited mechanical properties and are brittle and fragile, with a very low degradation rate in the body. On the other hand, the brittle nature of calcium phosphate ceramics limits their use alone. The bone of the common cuttlefish (*Sepia officinalis*) is primarily composed of a mineral compound known as calcium carbonate. Calcium carbonate, by itself, does not possess desirable mechanical strength and cannot be directly used to enhance the mechanical properties of cement. Additionally, the main mineral components of bone are derived from calcium phosphate compounds. In this project, the conversion of calcium carbonate obtained from the bone tissue of fish into calcium phosphate, the main mineral component of body bone, was carried out using a hydrothermal method. Finally, the compressive strength and biocompatibility of the cement were evaluated using MTT toxicity testing. Based on the results of XRD, SEM, and FTIR, it was shown that natural aragonite from squid bone was hydrothermally converted into hydroxyapatite. SEM images of composite samples showed that hydroxyapatite was well mixed with poly-caprolactone. The results obtained from the biocompatibility test showed that the bone cement composite reinforced with squid bone did not have toxic properties. Besides, the results of compressive strength tests showed that adding hydroxyapatite powder to bone cement could improve the mechanical properties of the composite. The results showed that increasing the percentage of hydroxyapatite powder improves the compressive strength and decreases the injectability of bone cement. Accordingly, this composite can serve as an appropriate alternative for use in the repair and reinforcement of weak and damaged bones.

***Keywords:*** Hydroxyapatite, Hydrothermal treatment, Bone cement, Compressive strength, *Sepia Officinalis*

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**Bioinformatic analysis of EF-TU receptor stability in Arabidopsis**

Mehdi Safaeezadeh, Masoumeh Fallah Ziarani

**Abstract**

EF-TU is the elongation phase factor and plays an important role in the expression of proteins. Due to the importance of this protein in the translation process, the stability of this protein was investigated. The results showed that this protein is one of the unstable proteins.

***Keywords:*** EF-TU, Sustainability, translation

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**Enzyme kinetics in *ficus* *carica*.l,** **cv. ‘sabzʼ**

Mansoore Shamilia,\*, Razie Esfandiari Ghalatib

**Abstract**

There is a growing request for enzymes in the universal market. Proteases are among the most industrial commanded enzyme, included animal proteases (trypsin and pepsin), microbial proteases (bacterial, fungal and viral proteases) and plant proteases (papain and ficin). The upward requirement for biologic-based enzymes, in the food industry, made them an interesting subject for biochemists. But, their sensitivity to extreme conditions causes some restrictions. We examined the fig leaf protease stability at a range of pH (2, 3, 4, 5, 6, 7, 8) and temperature (30, 40, 50, 60, 70, 80 and 90 °C). According to our result, the optimal temperature for fig leaf proteases activity was 30 °C. The optimal pH for the leaf extract protease activity was 4. The findings revealed protease obtained from fig is a probable candidate to be used as a natural food stabilizer.

***Keywords:*** Enzyme stability, Fig, pH stability, Protease activity, Thermal stability

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**Anthocyanin stability kinetics in *Ficus* *carica*.L, cv. ‘Shah anjirʼ**

Mansoore Shamilia,\*, Razie Esfandiari Ghalatib

**Abstract**

Anthocyanins are water-soluble pigments bringing a distinct color, from pink, red, violet, to dark blue (by pH rises). Anthocyanins are present at high concentrations in various plant derived products. Anthocyanins noticed for their potential anti-oxidant and anti-inflammatory activities to improve human health and reduce risks of diseases. One of the main limits the industrial application of anthocyanins is their instability during storage and processing. The degradation of anthocyanins during thermal process and storage can be enhanced by light conditions. In the present research, fig leaf extract was studied to examinate the thermal stability of anthocyanins. To extract leaf anthocyanin leaves were ground with acidic methanol and the absorption was read at 530 and 670 nm. Extract containing anthocyanins was heated (10, 20, 30, 40, 50, 60, 70, 80, 90 and 100ºC) under different pH (2, 3, 4, 5 and 6) and light conditions (light and dark). Fig anthocyanin extracts were more stable under pH 4 and 5, temperature 20 and 30° C, both dark and light conditions. The findings revealed fig anthocyanin is a probable candidate to be used as a natural food colorant*.*

***Keywords:*** Anthocyanin, Temperature, Light, pH

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**The effect of a non-ionic detergent on *Pseudomonas* lipase activity, kinetics and molecular dynamics studies**

Dariush Minai-Tehrani\*, Fatemeh Seyedmorad

**Abstract**

Lipases are indeed valuable enzymes in the industry, particularly in the production of washing powder where they play a crucial role. Bacterial lipase, especially from *Pseudomonas*, is of particular interest due to its high activity and potential for genetic modification. The interaction between lipase and detergents has been a subject of inquiry, leading to a research study on the effect of Triton X-100 on *Pseudomonas* lipase. Both *in- silico* and *in- vitro* methods were employed in this investigation. The *in-silico* results revealed that Triton X-100 can bind to a specific region outside the enzyme's active site, leading to hydrophobic interactions with phenylalanines. In the laboratory (*in- vitro*), it was observed that the enzyme exhibited its highest activity in the presence of detergent, particularly at the concentration bordering between the monomer and micelle state of the detergent. Furthermore, the presence of detergent caused a shift in the optimum pH and temperature for the enzyme. The fluorescence spectrum analysis supported the *in-silico* findings, demonstrating a change in the emission spectrum indicating the transfer of aromatic amino acids to a more hydrophilic environment in the presence of detergent. Overall, the research findings confirmed that lipase remains fully active in the presence of non-ionic detergent, while also highlighting the potential for detergents to alter the physico-chemical properties of the enzyme. These insights contribute to our understanding of the behavior of lipase in the presence of detergents, with implications for industrial applications.

***Keywords:*** Enzyme, Bacteria, Detergent, Activity, Molecular dynamics

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**Principles of Droplet-based digital PCR and its applications**

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**Abstract**

Nucleic acids are crucial targets for analysis across diverse fields, including medicine, food safety, and environmental science. the polymerase chain reaction (PCR) and its derivatives have emerged as transformative tools in biological and diagnostic applications. As an innovative advancement in the realm of absolute quantitative polymerase chain reaction methodologies, the droplet-based digital PCR (ddPCR) technique offers a multitude of advantages including exceptionally high sensitivity, remarkable precision and outstanding reproducibility, which are critical parameters in the realm of molecular diagnostics. in light of the burgeoning demand for point-of-care (POC) detection and clinical diagnostics, a low-cost, portable, and user-friendly droplet-based digital PCR device has emerged as an intriguing focal point of research, attracting significant attention from the scientific community. Given its extraordinary potential for seamless integration and advanced miniaturization, microfluidic technology has been proficiently utilized across a diverse range of digital droplet polymerase chain reaction (ddPCR) methodologies, significantly augmenting both their operational efficiency and overall practicality in various applications.

***Keywords:*** PCR, Droplet-based digital PCR, qPCR, Applications

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**Optimizing Zeolitic imidazolate frameworks-8 (ZIF-8) nanocomposite for Quercetin loading efficiency**

Zahra Jafari, Somayyeh Ghareghomi, Ali Khatibi\*

**Abstract**

Cancer is the second most common cause of mortality worldwide. Advanced drug delivery systems offer a targeted and efficient approach for improving cancer therapy outcomes while minimizing side effects. Zeolitic imidazolate frameworks (ZIFs) constitute a category of metal-organic frameworks (MOFs) distinguished by a zeolite-like architecture and the incorporation of imidazolate linkers. Zn2+-based ZIF (ZIF-8) has garnered considerable attention within the biomedical domain owing to its minimal toxicity and favorable biocompatibility profile. Quercetin (Que) stands out as the most prevalent flavonoid, exhibiting potent antioxidant properties and a multitude of biological functions, including antimicrobial, antidiabetic, anticancer, and anti-inflammatory activities within the biomedical sphere. By conducting research, the Mechanochemical method was used for ZIF-8 nanocomposite at different times (8, 16, 24 h), while the amount of initial materials was the same in all three times. Proceeded the Que loading as a pharmacological agent at ratios of 1:1 and 2:1 (ZIF-8: Que). Based on the obtained results, the efficiency of ZIF-8 synthesis is directly dependent on the time of synthesis. Also, drug loading at lower ratios of quercetin, yielded superior outcomes.

***Keywords:*** Antioxidant, Drug delivery, Optimization, Quercetin, Zeolitic imidazolate frameworks (ZIFs)

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**Clustering the generalized binding region of beta-secretase for Alzheimer's drug design**

Sajedeh Bahonar

**Abstract**

Beta-secretase-1 (BACE-1), a type I transmembrane aspartic protease, is a critical enzyme involved in the pathology of Alzheimer’s disease, making it a prime target for therapeutic intervention. The identification and characterization of its Generalized Binding Region (GBR) provide crucial insights into ligand-protein interactions, aiding in drug design. By leveraging structural data and computational approaches, this study aims to define the GBR of BACE-1, analyze its structural conformations, and cluster these conformations for efficient ligand-binding studies. Thirteen BACE-1 protein-ligand complexes were obtained from the Protein Data Bank (PDB) and processed using VMD software to clean and extract relevant structural data. The GBR was defined as residues within 4.5 Å of the ligands, and structural superposition was performed to minimize RMSD between equivalent residues. An RMSD-based dissimilarity matrix was calculated, and k-means clustering was applied to group the conformations into structurally homogeneous clusters. Representative complexes for each cluster were identified, and hydrogen atoms were added using Reduce software. All analyses were conducted using TCL scripts in VMD and statistical tools in R. The GBR analysis identified seven key residues (GLY11, GLN12, GLY13, LEU30, ASP32, GLY34, SER35) frequently interacting with ligands, predominantly located in beta-sheet and turn secondary structures. Clustering the complexes based on the RMSD matrix resulted in three distinct clusters, each represented by a conformationally unique structure. These representative structures provide a comprehensive view of the GBR, facilitating the reduction of docking experiments and offering a robust framework for targeted drug design. Further exploration of alternate conformations and contact thresholds could enhance the accuracy of GBR characterization, contributing to more effective inhibitor development for Alzheimer’s treatment.

***Keywords:*** Beta-secretase-1, Alzheimer’s disease, Generalized binding region, Structural clustering, RMSD, Drug design

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**Development of magnetic nanocomposites from shrimp shells**

Fatemeh Sedaghatia,\*, Tayebeh Kamali Zarkanib, Fayezeh Samarib,c

**Abstract**

Shrimp shell waste, a significant byproduct of the seafood industry, presents a substantial environmental challenge [1]. This study explores the valorization of this waste material into value-added products through the development of magnetic nanocomposites. Chitosan, a biodegradable and biocompatible polymer, was extracted from shrimp shells and subsequently was used as bio-based material for the synthesis of magnetic nanocomposite. The influence of various factors on the synthesis of magnetic nanocomposites was studied. The structural, morphological, and chemical properties of chitosan and the magnetic nanocomposite were investigated using Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), Scanning Electron Microscopy with Energy Dispersive X-Ray Analysis (SEM-EDX), Brunauer–Emmett–Teller (BET) and Vibrating-sample magnetometer (VSM). The resulting nanocomposites exhibited excellent magnetic properties and high surface area. The potential applications of these nanocomposites include wastewater treatment, drug delivery, and biosensing. This research provides a sustainable solution for shrimp shell waste management while offering promising opportunities for the development of advanced materials with diverse applications.

***Keywords:*** Shrimp shells, Chitosan, Waste material, Magnetic nanocomposite, Characterization

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**A novel NADPH-dependent nitrate reductase with tellurite reductase activity from heavy metal resistance bacteria, *Bacillus Licheniformis* strain ZT1**

Fariba Mollaniaa,\*, Nasrin Mollaniab, Fatemeh Taktazb,c

**Abstract**

The tellurium and tellurium-containing compounds have been used extensively in several ﬁelds such as electronics, optics and biosensor creation. Some reductase enzymes could reduce tellurite or tellurate to generate tellurium nanoparticles. In this work, the NADPH-dependent nitrate reductase enzyme with tellurite reductase activity was purified from *Bacillus licheniformis* strain ZT1 that resistant to some heavy metals. The Km and Vmax values of purified enzyme were 1.5 mM and 0.3 µmol/min, respectively. The enzyme exhibited its optimum activity at pH 9 and 45°C. Divalent cations, such as Mn2+, Ca2+ and Mg2+, had no effect on the activity, while similar concentrations of Cu2+ abolished the activity. N-ethylmalemide furthermore could completely inhibit the enzyme activity due to changes in enzyme conformation. In order to investigate correctly the effects of water-miscible organic solvents on the behavior of the enzyme, some organic solvents were selected for the investigation. The enzyme revealed 65% of its initial activity in the presence of Tween 80.

***Keywords:*** NADPH-dependent nitrate reductase, Tellurite reductase activity, Heavy metal resistance strain

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**Establishment of an orthotopic xenograft retinoblastoma nude mouse model by intravitreal injection of human RB Y-79 cells and histological follow up**

Parto Tarraha, Yahya Sefidbakhtb,\*, Fatemeh Suric,\*, Mozhgan Rezaeikanavib,\*, Firouzeh Hatamib\*, Sina Khosravib\*

**Abstract**

Retinoblastoma (RB), is the most frequent primary intraocular tumor in children which if left untreated, can cause death. Preclinical animal models that mimic molecular, genetic and cellular features of cancers are essential for studying cancer and searching for promising diagnosis and treatment modalities and can also help to understand tumor biology, screening of new drugs and studying new ways of drug administration. To develop animal models of retinoblastoma that accurately resembles metastatic and non-metastatic form of the human disease, we injected human retinoblastoma Y79 cells intravitreally in both eyes of 6 BALB/c nude mice (male,5 weeks old), The incidences of retinoblastoma were analyzed by hematoxylin/eosin (HE) staining. Additionally, one injected nude mouse was kept for a longer period of time in order to study histological examination for potential metastases. Eyes were monitored morphologically every week for five weeks, tumor growth resulted in swelling of the eyes in individual animals. 8 weeks after injection histological analysis was performed and showed that Y79 retinoblastoma cells formed intraocular tumors that were initially confined to the vitreous cavity. Tumors progressively invaded the retina, subretinal space and anterior chamber of the eyes. The model described here has several advantages. It is readily available, easily established, and easy to work with. The existence of an in vivo model may offer new opportunities for the further cellular and molecular analysis of a human intraocular tumor.

***Keywords:*** Retinoblastoma, Xenograft, Mouse model, Histology

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**Synthesis of new β-lactams contain anthraquinone and their molecular docking**

Maaroof Zarei\*, Raheleh Jamalinasab, Masoud Mohamadzadeh

**Abstract**

β-Lactam antibiotics are the most important antibacterial agents for human health and it began with the discovery of penicillin by Alexander Fleming in 1928. In addition, β-lactams are an important class of heterocyclic compounds due to their wide range of applications in other biological activities. With the alarming trends in bacterial resistance to many β-lactam antibiotics it has become necessary to synthesize novel β-lactams for bioassay of antibacterial activity and the need for drugs with more specific antibacterial activity. Therefore, the synthesis of the new β-lactams is the subject of extensive study. The anthraquinone and related compounds have been represented as a broad and growing family of bioactive molecules. Novel β-lactams contain anthraquinone on C-3 position were synthesized by ketene-imine cycloaddition and characterized by spectral data. Molecular docking studies were carried out by Autodoc software. Penicillin-binding protein 2a (PDB ID: 1VQQ) from methicillin-resistant Staphylococcus aureus strain used as a target which good binding interactions were observed. In- silicomolecular docking studies of novel β-lactam-anthraquinone hybrids showed moderate to excellent interactions. Some of the synthesized β-lactams have lower binding energy than penicillin G. The overall interaction may be attributed to the presence of β-lactam ring and anthraquinone moiety.

***Keywords:*** β-lactam, Anthraquinone, Antibacterial, Bacterial resistance, Molecular docking

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**The use of Cu nanoparticles stabilized by C. Tinctorius plant extract in the synthesis of β-lactams**

Maaroof Zarei\*, Fayezeh Samari, Nazila Askari

**Abstract**

Besides the extensive medical application with high importance of the β-lactam antibiotics, β-lactams (2-azetidinones)have also represented other biological activities. Due to biological application of 2-azetidinones and their utility as synthetic intermediates, several methods for the preparation of 2-azetidinones have been presented. One of the applicable methodologies for the synthesis of 2-azetidinones is the Kinugasa reaction. The Kinugasa reaction is the direct synthesis of β-lactams from copper acetylides and nitrones which provides some advantages including its optimal atom economy and its employment of readily accessible starting materials. Recently, nanoparticles have been widely used in various biological applications and organic reactions because of low toxicity, easy preparation without the need for filtration step, large surface area ratio and increase the efficiency of catalytic activity. Today, a considerable number of reports have shown that the addition of rhus and safflower in food or water can have valuable effects on human and animal health. Safflower has been used for a long time as a basis for dietary fat, food coloring, and Chinese medicines. The goal of our work is to produce Cu nanoparticles by Carthamus tinctorius extract through green synthetic pathways which has been used in the synthesis of β-lactams from nitrones and alkynes using Kinugasa reaction. Due to the presence of β-lactam ring and various substitutions, the products can exhibit antibacterial properties and other biological activities.

***Keywords:*** β-lactam, 2-azetidinone, Antibacterial, Cu nanoparticles, Kinugasa reaction

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**Investigating a novel bi-allelic mutation in HPD-like protein: Docking simulation insights and literature overview**

Fatemeh Vaghefia, Teymoor Khosravia, Farzaneh Motallebia, Yahya Sefidbakhtb, Morteza Oladnabic,\*

**Abstract**

Hereditary Spastic Paraplegia (HSP) is a rare neurodegenerative disorder characterized by progressive weakness and spasticity in the lower limbs. Mutations in the HPDL gene are associated with Spastic Paraplegia 83 (SPG83), an autosomal recessive form of HSP. Although HPDL mutations are known to contribute to SPG83, the molecular mechanisms underlying their role remain poorly understood, primarily due to the rarity of the condition. This study aims to investigate the genetic basis of HSP in two consanguineous families from Iran. Whole-exome sequencing (WES) was utilized to identify genetic variants in the probands. To assess the pathogenic potential of the identified variants in the HPDL gene, various computational tools such as SIFT, CADD, Mutation Taster, Polyphen-2, and PANTHER were employed. Conservation analysis of the HPDL protein sequence was conducted using Clustal Omega and ConSurf tools, while the 3D structure of HPDL variants was predicted using the I-TASSER server. Protein-protein interactions involving HPDL were explored through the STRING database. Additionally, the DynaMut web server was used to evaluate the impact of the identified mutations on protein dynamics and stability. The effects of the variants on protein stability were further assessed using the I-Mutant and MUpro web servers. Finally, protein-ligand docking simulations were performed using Molegro Virtual Docker (MVD), a state-of-the-art integrated platform. WES identified two biallelic missense mutations: c.3G>C (p.Met1Ile) and c.128G>A (p.Arg43Pro) in the HPDL gene. The c.128G>A mutation is novel and is reported here for the first time in a patient with SPG83. Trio-based co-segregation analysis confirmed the inheritance of these variants. A thorough literature review indicated a significant consanguinity rate (49.55%) among families with HPDL mutations. Additionally, based on ΔΔG predictions and protein flexibility analysis, it was found that the p.Arg 43Pro variant led to a reduction in molecular flexibility. This study reinforces the association between HPDL mutations and HSP, specifically SPG83. Moreover, our bioinformatics findings represent an initial step toward validating the identified variant as a pathogenic mutation, paving the way for future functional studies.

***Keywords*:** Hereditary spastic paraplegia, Spastic paraplegia 83, HPDL gene, Whole exome sequencing, Iran

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***in- silico* investigation of PAH gene mutations in Iran: Identification and docking simulation of potential pathogenic variants**

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**Abstract**

Phenylketonuria (PKU) is the most prevalent inherited metabolic disorder resulting from a malfunction in the phenylalanine hydroxylase (PAH) enzyme. The diverse and consanguineous nature of the Iranian population offers a valuable opportunity to investigate autosomal recessive disorders. We investigated 159 mutations in the PAH gene reported in Iran using various computational approaches. Pathogenicity and stability of genetic variants were assessed using tools like ACMG, Fathmm, CADD, SIFT, PolyPhen-2, Mutation Taster, MUpro, and I-Mutant 2.0. Amino acid conservation was analyzed with Clustal Omega and Consurf web servers. Secondary and tertiary modeling of wild-type and mutant PAH enzymes was performed using PSIPRED and I-TASSER, respectively, and 3D structures were visualized with PyMOL. Protein-protein interactions were explored using the STRING database, and potential pathogenic variants were identified through the Iranome Genomic Database. Additionally, we conducted protein-ligand docking simulations with Molegro Virtual Docker (MVD) to evaluate the structural and functional consequences of the putative pathogenic mutation (c.688G>A). Our analysis revealed that 80.8% of mutations occur in conserved regions, especially within the catalytic domain, with nearly half being missense mutations. The c.688G>A variant was identified as a putative pathogenic mutation according to the Iranome Genomic Database. The cohort had a consanguinity rate of 31.67%. Docking studies indicated that this variant results in a significant loss of a catalytic site residue in the catalytic domain. PCR sequencing was the most common genetic testing method, accounting for 71.5% of cases. This study provides insights for future functional research, genetic counseling, and the development of diagnostic tools, including a strip assay kit.

***Keywords:*** PAH Gene, Phenylketonuria, Iran, Spectrum of mutation.

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**Flavonoids as inhibitors of amyloidogenic protein fibrillation: Identification and evaluation of candidates**

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**Abstract**

In recent years, herbal treatments have garnered more attention due to their low cost and fewer side effects. Flavonoids, as one of these compounds, can reduce the aggregation of amyloidogenic proteins. This study aims to identify flavonoids with the greatest impact on inhibiting the fibrillation of amyloidogenic proteins associated with neurodegenerative diseases such as Parkinson's and Alzheimer's. In the first phase, 98 flavonoids were selected from various databases and examined, ultimately leading to the selection of 46 as preliminary candidates. This selection was based on the effectiveness of flavonoids in inhibiting the aggregation of amyloidogenic proteins that were approved in previous research. Subsequently, using the OSIRIS and Swiss ADME web servers, toxicity, mutagenicity, drug-likeness, and their ability to cross the blood-brain barrier was evaluated. Some candidates were excluded from further consideration due to non-compliance with these criteria. Docking studies using Vina-dock showed interactions between flavonoids and amyloidogenic proteins at potential binding sites identified by the DoGSiteScorer and CASTp web servers. The amino acids involved in binding were determined using Ligplot and PLIP. Ultimately, flavonoids that exhibited the lowest binding energy and interacted with amino acids at identified amyloid hot spots by FoldAmyloid, TANGO, and Waltz web servers were chosen for *in- vitro* analysis. In this stage, alpha-synuclein was incubated under fibrillation conditions in the presence and absence of flavonoid treatments. Results from Thioflavin-T fluorescence assays, atomic force microscopy, and enzymatic digestion tests with proteinase K indicated that certain flavonoids could significantly inhibit the formation of alpha-synuclein fibrils. Fourier-transform infrared spectroscopy also demonstrated a reduction in β-sheet content, confirming the inhibitory effects of these flavonoids. Cell culture studies revealed that these flavonoids increase the survival of neuronal cell lines treated with alpha-synuclein fibrils.

***Keywords*:** Flavonoid, Beta-amyloid, Alpha-synuclein, Neurodegenerative diseases

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**A bioluminescent molecular switch for label-free detection of SARS-CoV-2**

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**Abstract**

Bioluminescent proteins, especially photoproteins like aequorin, have gained significant attention for their ability to emit light upon binding with specific ions, such as calcium. This unique property makes photoproteins highly effective in biosensor applications, enabling precise and sensitive detection of biological targets [1-3]. Amid the ongoing global challenge of SARS-CoV-2 in 2024, the need for advanced diagnostic tools is critical. Aequorin-based biosensors stand out due to their rapid response, real-time detection capabilities, and exceptional sensitivity, offering a powerful approach for detecting viral components and managing the spread of COVID-19[4,5]. This study focuses on the design of AeqACE2, a fusion protein combining aequorin, with an ACE2-driven peptide for the detection of SARS-CoV-2, which is known to bind to the spike protein of SARS-CoV-2. The protein construct was expressed in *E. coli* BL21(DE3) cells as inclusion bodies. After the refolding process, the protein was successfully recovered in a soluble form suitable for further characterization. Circular dichroism spectroscopy was employed to assess the secondary structure of the refolded protein. We evaluated the bioluminescent emission of the AeqACE2 in the presence and absence of SARS-CoV-2. The results showed a significant increase in bioluminescent intensity in the presence of the virus, confirming that the construct acts as a molecular switch. Control experiments with non-specific proteins and virus-free conditions demonstrated minimal or no change in luminescence, highlighting the specificity of AeqACE2 for SARS-CoV-2. Quantitative analysis revealed a dose-dependent increase in bioluminescent emission with increasing concentrations of SARS-CoV-2, demonstrating the sensitivity of the biosensor. Additionally, the protein's rapid response to the presence of the virus supports its potential for real-time detection. In conclusion, the successful design and expression of this switch demonstrate its potential for use in a highly sensitive biosensor for the detection of COVID-19, providing a promising diagnostic tool in the ongoing fight against it.

***Keywords:*** Bioluminescent proteins, Photoprotein, COVID-19 detection, Protein switch, Aequorin, SARS-CoV-2

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**The investigation of the effect of SUMO (Small Ubiquitin-like Modifier) on the inhibition of fibrillation in alpha-synuclein and beta-amyloid proteins**

Khosro Khajeh\*, Bahareh Dabirmanesh, Hamid Saedi

**Abstract**

The study of protein fibrillation and the development of strategies to prevent this process has garnered significant attention in recent years. The role of SUMO (Small Ubiquitin-like Modifier) protein as a chaperone in the solubility of amyloid fibrils and its ability to inhibit protein fibrillation has been demonstrated in previous research. This study investigates the fibrillation of alpha-synuclein and beta-amyloid proteins in the presence and absence of SUMO. The formation of amyloid fibrils was assessed using Thioflavin T (ThT) fluorescence emission at a wavelength of 485 nanometers. The results were corroborated through various techniques, including Atomic Force Microscopy (AFM), Circular Dichroism (CD) spectroscopy, Fourier Transform Infrared (FT-IR) spectroscopy, and Congo Red absorbance analysis. In all samples under fibrillating conditions, the absence of SUMO resulted in a significantly higher formation of amyloid plaques, whereas the presence of SUMO led to a marked reduction in their formation. The findings from this study confirm the role of SUMO as a chaperone in dissolving fibrillated amyloids.

***Keywords:*** SUMO, Fibrillation, Beta-amyloid, Alpha-synuclein

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**Evaluation of α-amylase enzyme immobilization upon chitosan polymer for the evaluation of biosensors synthesis**

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**Abstract**

Enzymes, as biological catalysts, play a pivotal role in numerous biological and industrial processes. Their extensive applications in medicine, food industries, biotechnology, and environmental science include drug production, environmental pollutant degradation, chemical reaction optimization, and the fabrication of diagnostic biosensors. However, the direct utilization of enzymes faces challenges such as low stability, limited activity under unfavorable conditions, and difficulties in recovery and reuse. An effective strategy to address these issues is enzyme immobilization onto suitable supports, which enhances stability, improves efficiency, and facilitates recovery. In this study, the immobilization of alpha-amylase enzyme onto a chitosan polymer support was investigated. Chitosan, a biocompatible and biodegradable polymer, is considered a suitable choice for this purpose. Covalent bonding, along with a crosslinking agent (glutaraldehyde), was employed to attach the enzyme to the support. The experiments demonstrated that the enzyme activity remained within the standard range post-immobilization, and its stability under environmental conditions was improved. Furthermore, structural analyses using XRD confirmed that the immobilization process did not negatively impact the enzyme's structure. The findings of this research indicate that enzyme immobilization onto biocompatible polymer supports not only enhances their performance but also enables reuse and reduces economic costs. This method can find broad applications in the pharmaceutical industry, bioremediation, and industrial enzyme production.

***Keywords:*** Immobilization, Enzyme activity, α-amylase, Chitosan

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**The effect of deep eutectic solvent on the stability of ICD-TDP-43 protein liquid droplets**

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**Abstract**

The distinctive characteristics of deep eutectic solvents (DESs) offer the potential to stabilize proteins. They can prevent the aggregation of proteins, such as LCD-TDP-43, which serves as a model for prion-like protein [1]. Essentially, DESs impede denaturation caused by external stressors by encapsulating proteins within a protective barrier [2]. DESs fulfill their function by enhancing solvation around proteins, reducing hydrophobic interactions, and maintaining protein structure during phase separation [3.4]. This study aims to develop and refine DES formulations to enhance protein stability during the phase separation pathway [5]. In this study, the pJ-411 vector was used to express the recombinant LCD-TDP-43 protein in *E. coli* BL21 (DE3). Affinity chromatography with Ni-NTA was employed to purify the protein. Dialysis was used to study phase transitions from liquid droplets to amyloid fibrils. After 72 hours of dialysis, the LC domain transitioned from liquid droplets to amyloid fibrils. Liquid-liquid phase transitions occurred first, followed by liquid-solid phase transitions, with a white precipitate indicating amorphous mature droplets and amyloid fibrils. Five DESs were prepared to investigate their effect as chemical chaperones on the aggregation process of LCD-TDP-43 protein. These DESs included betaine: glycerol (1:2), betaine: sorbitol (1:2), betaine: citric acid (1:1), betaine: tartaric acid (1:1), and betaine: xylose (1:2). Protein aggregation in the phase separation pathway was examined, and amyloid fibrils were identified using turbidity measurements and ThT fluorescence. Turbidity measurements revealed a decrease in UV-visible absorption in the presence of several DESs, indicating their potential role in inhibiting amyloid growth in LCD-TDP-43 proteins. This finding suggests that DESs may play a crucial role in improving protein stability during liquid-phase separation. Consequently, DESs may be considered as promising candidates in the search for new therapeutic agents to treat diseases associated with protein aggregation.

***Keywords:*** DESs, LCD-TDP-43, LLPS, Protein aggregation, Neurodegeneration, ALS

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**Exploring anti-cancer drugs membrane permeation: A molecular dynamics study using umbrella sampling**

Sheyda Zarghami, Yahya Sefidbakht\*

**Abstract**

This study examines how anti-cancer drugs permeate lipid bilayers using molecular dynamics simulations with umbrella sampling techniques. We investigate how different lipid compositions affect membrane interaction and transport of these therapeutics to optimize drug delivery systems. We analyze both hydrophilic and hydrophobic anti-cancer agents across varying membrane compositions including phosphatidylcholine, sphingomyelin, and cholesterol.Using umbrella sampling, we calculate the potential of mean force associated with drug insertion into lipid bilayers, providing insights into the free energy landscape of drug-membrane interactions. We define a reaction coordinate based on the distance between the drug molecule and the bilayer's center of mass, creating multiple overlapping windows to enhance sampling efficiency and capture conformational changes and energy barriers during permeation.Our findings show that lipid composition significantly influences drug permeability, with certain lipid environments either facilitating or hindering drug translocation. Our simulations reveal distinct variations in the free energy landscape based on drugs' physicochemical properties. Smaller, more hydrophobic drugs exhibited lower energy barriers, facilitating permeation compared to larger, polar compounds.The results highlight the importance of umbrella sampling in molecular dynamics studies for accurately characterizing complex interactions between anti-cancer drugs and lipid membranes. This research deepens understanding of drug delivery mechanisms and may inform more effective anti-cancer therapy design by optimizing membrane permeation properties..

***Keywords:*** Molecular dynamics, Lipid bilayers, Anti-cancer drugs, Umbrella sampling, Permeation, Drug delivery

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**Fabrication of an optical sensor using green-synthesized Urtica dioica-derived carbon quantum dots for iron (II) detection**

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**Abstract**

Carbon Quantum Dots (CQDs), due to their wide range of sources and their features such as fluorescence emission, have shown many different incredible applications in the past years. In this study, hydrothermal method, as a reliable and low-cost method, was used for green synthesis of CQDs from *Urtica dioica*. For the hydrothermal process, 1.5 g of the plant was powdered and mixed with 30 ml of water. After that, the solution was sonicated for 30 min at the room temperature (25 °C). The solution was then transferred into a hydrothermal reactor and was placed and heated in an oven at 250 °C for 6 h. The resulting solution was then allowed to cool down to room temperature. The synthesized CQDs were purified in 3 steps, first by Whatman filter paper, after that, they were centrifuged at 20000 rpm for 20 min, and at last, by 0.22µm syringe filter. The synthesized CQDs were then used as a probe for metal detection against 10 mM of Cu (II), Hg (II), Pb (II), Fe (II), and Fe (III). Fluorescence quenching studies revealed that these CQDs can be used as an optical sensor for detecting trace amounts of iron (II) ions.

***Keywords:*** Graphene quantum dots, Optical sensor, Photoluminescence, Hydrothermal

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**Probing electroporation in lipid bilayers: Insights from molecular dynamics simulations**

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**Abstract**

Electroporation is a critical phenomenon in cellular processes, where applied electric fields induce transient pores in lipid bilayers, facilitating molecular transport. This study aims to elucidate the underlying mechanisms of electroporation at the molecular level, using advanced molecular dynamics simulations to model the effects of specific electric field strengths ranging from 10 to 100 MV/m on various lipid bilayer compositions. By systematically varying the electric field intensity and lipid types, we investigated the dynamics of lipid rearrangements, pore formation, and stabilization. Our simulations revealed that fields exceeding 50 MV/m significantly enhanced pore formation, with distinct differences observed based on lipid saturation and headgroup structure. Furthermore, we characterized the critical transition points for pore emergence, highlighting the role of lipid packing and hydrophobic mismatches in modulating electroporation susceptibility. These findings provide a comprehensive understanding of how electric fields interact with lipid membranes, offering insights that could enhance applications in drug delivery and gene therapy. The results underscore the importance of optimizing electric field parameters for efficient electroporation, paving the way for future experimental validations and practical applications in biotechnology and membrane biophysics.

***Keywords:*** Electroporation, Molecular dynamics, Lipid bilayers, Electric fields, Pore Formation, Membrane Permeability

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**Investigating the role of Sumo tag in fibrillation of bacterial lipase**

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**Abstract**

Interest in the formation of amyloid by peptides and proteins has increased significantly in recent years and has attracted a lot of attention due to its application in protein chemistry, biotechnology, biology and medicine. This process typically consists of three characteristic stages: a lag, a growth and a plateau phase. In this study, the formation of amyloid fibrils from microbial lipase of pseudomonas strain was performed under conditions that are close to the physiological state, in the presence and absence of sumo tag. Since the sumo tag is used to increase the expression and solubility of the recombinant protein, for this purpose, in this study, two gene constructs with sumo sequence and without sumo sequence were designed. Cloning, expression and purification of these two gene constructs were performed, then the formation of amyloid fibrils after diluting urea with thioflavin T (ThT) fluorescence methods, Congo red binding, dynamic light scattering, rotational spectroscopy and Fourier transform infrared spectroscopy and Fourier transform infrared spectroscopy, X-ray scattering and atomic force microscopy imaging (AFM) was checked. The results of this investigation show that the aggregates formed in the structure without sumo compared to the structure with sumo show an increase in the number of beta sheets and the formation of lipase fibrils takes place immediately after dilution in the first few seconds in the structure without sumo, but in the structure with sumo sequence, no amyloid fibril was formed, which indicates that the sumo sequence probably plays a role in the non-formation of amyloid fibrils.

***Keyword:*** Amyloid fibrils, Lipase, Sumo tag, Rapid aggregation

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**Inducing robust humoral and mucosal immunity against SARS-CoV-2 using yeast surface display system**

Tahereh Saveiia, Sareh Arjmandb, Ismaeil Haririanc Reza H. Sajedia,\*

**Abstract**

The SARS-CoV-2 virus, the causative agent of the COVID-19 pandemic, has become a serious global health threat. The receptor-binding domain (RBD) of the spike protein is a critical component of the virus, essential for its entry into human cells, and a prime target for vaccine development. In this study, we aimed to enhance humoral and mucosal immunity by developing recombinant *P. pastoris* yeast displaying the RBD on its surface using the SEDI anchor. The RBD gene was synthesized and electroporated into competent *P. pastoris* cells. After screening positive clones on PAD plates, *P. pastoris*/pPink-αHC-RBD-SEDI was cultivated in BMGY medium and subsequently induced in BMMY medium. The surface expression of the RBD protein was confirmed using ELISA, flow cytometry, and immunofluorescence assays. Oral immunization was administered to mice on days 1 and 2 for primary immunization and on days 14 and 15 for booster immunization. Blood and fecal samples were collected on day 28. ELISA results indicated that the absorbance at 450 nm for yeast expressing RBD was twice as high as that of the control yeast. Mice administered with RBD-expressing yeast exhibited higher serum IgG levels compared to those receiving control yeast. Fecal IgA levels were also elevated in mice treated with RBD yeast compared to the control group, indicating enhanced mucosal immunity. Our findings underscore the significance of the RBD as a key target for SARS-CoV-2 vaccine design and provide evidence for the efficacy of an orally administered yeast-based SARS-CoV-2 vaccine in inducing robust immune responses. Importantly, the yeastsurface display system could serve as a universal technological platform for the development of other oral vaccines.

***Keywords:*** *p. pastoris*, SARS-CoV-2, Receptor-binding domain (RBD), Immune response, Yeast surface display

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**Structural adaptation of late embryogenesis abundant protein from *Artemia* under molecular crowding conditions**

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**Abstract**

Late embryogenesis abundant (LEA) proteins are crucial for protecting organisms like *Artemia* against abiotic stresses, such as high salinity and drought [1,2]. Although their protective roles are well-documented, the underlying molecular mechanisms, particularly regarding their structural adaptations under stress, remain poorly understood. This study investigates the structural behavior of LEA proteins in response to molecular crowding agents and membrane mimetics, which replicate conditions similar to those encountered during environmental stress. LEA protein from *Artemia urmiana* was expressed in *E. coli* BL21(DE3) and purified. To mimic the molecular crowding and stress conditions, we selected compounds such as polyethylene glycol (PEG), glycerol, trifluoroethanol (TFE), and sodium dodecyl sulfate (SDS). PEG and glycerol simulate molecular crowding, while TFE induces the formation of helical structures, and SDS serves as a membrane mimic, as LEA proteins are known to protect cell membranes under stress [3,4,5]. We used spectroscopic techniques-UV absorption, circular dichroism (CD), and fluorescence spectroscopy-to examine the structural transitions of LEA proteins in the presence of these compounds. Our results show that in its native, hydrated state, the LEA protein predominantly adopts a random coil conformation. However, in the presence of PEG, glycerol, and TFE, the protein underwent a structural shift toward increased helicity, indicating a transition to a more compact conformation. This helical formation was most pronounced in the presence of TFE, suggesting that LEA proteins may utilize such structural changes to stabilize cellular structures under stress. Additionally, in the presence of SDS, which mimics a membrane environment, LEA proteins showed enhanced folding, supporting their known membrane-protective role.

***Keywords:*** LEA proteins, Molecular Crowding, Trifluoroethanol, SDS, Artemia

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**Effect of exosomes on retinoblastoma cancer cells in drug delivery**

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**Abstract**

Exosomes are extracellular vesicles secreted by almost all cell types, playing a significant role in cell-to-cell communication and in transporting therapeutic agents and biomolecules such as proteins and RNA. Mesenchymal stem cell-derived exosomes have attracted attention due to their unique characteristics, including low toxicity, biocompatibility, and minimal immune response. On the other hand, doxorubicin is a chemotherapy drug widely used to treat various cancers, including retinoblastoma—a common intraocular cancer in children caused by mutations in the RB1 gene. In this research, exosomes derived from mesenchymal stem cells were employed to deliver doxorubicin to retinoblastoma cancer cells in order to investigate their effects. Exosomes were isolated from Wharton jelly mesenchymal stem cells using size-exclusion chromatography. They were then loaded with doxorubicin by sonication, and the effect of exosomes, drugs, and doxorubicin-loaded exosomes on Y-79 cells was examined through an apoptosis assay. The results indicate that the exosomes alone exhibited no toxicity toward the cancer cells, while the combination of exosomes and the drug showed enhanced induced apoptosis compared to the drug alone.

***Keywords:*** Exosome, Retinoblastoma, Drug delivery

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**Investigation of the interaction of human α-1-acid glycoprotein ~~(AGP)~~ with copper oxide nanoparticles ~~(CuO NPs)~~**

Sara Asgari, Fakhrossadat Mohammadi\*

**Abstract**

Nanoparticles in the diameter range of 1-100 nm show physical properties that can be completely different from the bulk metal. The parameters such as the size of the particles, the nature of the protective organic layer on the nanoparticles surface, and the shape of the nanoparticles affect the nanoparticles properties. It is now well accepted that when nanoparticles come into contact with a biological environment, their surface is covered by biomolecules such as proteins, and amino acids. The adsorbed protein layer on the surface of nanoparticles is called protein corona. Alpha-1-acid-glycoprotein, AGP, is one of the positive acute-phase proteins of all mammals. Copper oxide nanoparticles, CuO NPs, are one of the most important intermediate metal oxides nanoparticles, which have unique physicochemical properties. Copper oxide nanoparticles have attractive properties such as high stability, biocompatibility, and high absorption of visible light. In this study, we have synthesized and characterized the CuO NPs and further their cytotoxicity against the normal cells were investigated. The formation of protein corona upon interaction of AGP protein with CuO NPs have been studied using cyclic voltammetry method. According to the results, the redox peak currents decreased considerably and the redox peak potentials shifted which indicating the adsorption of the AGP molecules on the surface of CuO NPs. The binding constant of the formed protein corona of AGP estimated from the cyclic voltammogram showed the high affinity of AGP to adsorb on the surface of CuO NPs.

***Keywords:*** Copper oxide Nanoparticles,Human α-1-acid glycoprotein (AGP), Protein corona, Cyclic voltammetry

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**Study on achieving a drug that controls depressive disorders by inhibiting the enzyme monoamine oxidase A**

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**Abstract**

Depression is one of the acute neurological disorders that affects many people in Iran and around the world every year. The level of activity of the monoamine oxidase A enzyme plays a role in the development of depression-related disorders, including various psychological abnormalities. This study evaluated several ligands susceptible to inhibiting the monoamine oxidase A. First, these enzyme ligands were selected, and their three-dimensional structures were prepared from the PubChem structural database. Also, the three-dimensional structure of the monoamine oxidase A was prepared from the PDB protein database. Then, the molecular docking process was performed after preparing the ligand and the receptor to examine their interaction. The results of this study showed that these derivatives exert various effects in inhibiting the monoamine oxidase A by their structural characteristics. Therefore, from the study of the changes in the desired chemical structure among the investigated derivatives, dextroamphetamine (L5) is introduced as one of the most important selegiline derivatives in inhibiting monoamine oxidase A.

***Keywords:*** Monoamine oxidase A, Neurological diseases, Molecular docking, Dextroamphetamine

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**Enhancement of thermostability of *Aspergillus flavus* urate oxidase by site-directed mutagenesis**

Asal Banoo Familia, Bahareh Dabirmaneshb, Khosro Khajehb, Azadeh Ebrahim Habibic,\*

**Abstract**

Uricase (EC 1.7.3.3; Uox) is a peroxisomal oxidoreductase that catalyzes the oxidation of uric acid to hydrogen peroxide and allantoin. Its absence in humans leads to elevated uric acid levels (hyperuricemia) due to the consumption of high-protein foods, ultimately resulting in diseases such as gout. Therefore, uricase is utilized as a therapeutic enzyme for treating hyperuricemia-related conditions. This study aims to enhance the thermal stability of uricase through targeted mutagenesis via genetic engineering. Initially, molecular dynamics simulations (*in- silico*) were performed to analyze protein unfolding. By comparing parameters such as energy, radius of gyration, RMSD, and RMSF between candidate mutations and the wild-type enzyme, an optimal mutation was selected. Mutagenesis was conducted using targeted mutagenesis techniques, followed by optimization of enzyme transformation and expression in E. coli, with purification achieved through nickel affinity chromatography. The expression and purity of the enzyme were confirmed using SDS-PAGE, showing a molecular weight of 43 kDa for uricase in vertical electrophoresis. This study will evaluate the activity of both the mutated and wild-type enzymes and comparing their thermal stability.

***Keywords:*** (Root-Mean-Square-Deviation) RMSD، (Root-Mean-Square-Fluctuation) RMSF, Radius of gyration, Molecular dynamics simulations

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**Design and fabrication of nanocomposite hydrogel based on polyacrylic acid containing cellulose nanocrystal and zinc sulfide nanoparticles for wound dressing application**

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**Abstract**

Hydrogels are biomimetic materials that mimic the extracellular matrix of biological soft tissues. Due to that fact, the use of hydrogels in biomedical applications has become a rapidly expanding research area in biomedical field. Fabrication of a wound dressing that simultaneously has proper biological and mechanical properties is a challenging issue. The aim of this work is to exploit of nanomaterials to endow appropriate mechanical and biological properties to polyacrylic based hydrogel for wound dressing application. For this purpose, the Hydrogel was synthesized with polyacrylic acid (PAA) as the base polymer, including cellulose nanoparticles and zinc sulfide nanoparticles. Cellulose nanoparticles were considered to improve the mechanical properties and zinc sulfide nanoparticles to give antibacterial properties to the wound dressing. Analysis such as SEM, FTIR, and TGA were conducted for characterizing the hydrogel. MTT assay confirmed that the wound dressing is biocompatible. Animal study demonstrated that the hydrogel significantly promotes the healing of full-thickness skin defects in the rat model. In addition, microbiological analysis showed that the wound dressing has significant antimicrobial activity against Staphylococcus aureus and Escherichia coli. Our work introduces a biocompatible, antimicrobial hydrogel that may have promising clinical applications as a wound dressing material.

***Keywords:*** Hydrogel, Wound dressing, Poly acrylic acid, Zinc sulfide nanoparticle, Cellulose nanocrystal

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**Biomolecules-incorporated marine bio ceramic-based nanomaterials for drug localized delivery**

Sara Jamshidizadeh, Narges Amrollahi biuki\*

**Abstract**

The use of both manmade and natural materials for repairing and reconstructing bodily organs and tissues has a long history dating back to prehistoric times. However, in recent decades, there has been a significant acceleration in their utilization in scientific research and clinical applications. The advanced processing methods and new chemical strategies allow the incorporation of drugs within them or on their functionalized surfaces. In this regard, bio ceramics act as local [drug delivery systems](https://www.sciencedirect.com/topics/pharmacology-toxicology-and-pharmaceutical-science/drug-delivery-system) to treat large [bone defects](https://www.sciencedirect.com/topics/pharmacology-toxicology-and-pharmaceutical-science/bone-defect), [osteoporotic fractures](https://www.sciencedirect.com/topics/pharmacology-toxicology-and-pharmaceutical-science/fragility-fracture), bone infections and bone tumors. The importance of understanding implant-tissue interactions on a nanoscale level has led to the widespread use of nanotechnology in the field of biomedical science and engineering. This is supported by the idea that nanostructured materials can be customized and integrated into various biomedical implants and devices. Additionally, natural nanostructured patterns can be observed in biological systems like membranes, viruses, and protein complexes, while intricate architectural designs with interconnected open pores can be found in marine environments. Utilizing naturally-occurring marine skeletons offers promising solutions for advancing research and development in regenerative medicine for dentistry and orthopedics. These materials provide abundant supplies of osteopromotive analogues, biomineralization proteins, and a variety of framework designs and devices. Marine organisms, whether used in their original form or transformed into materials suitable for human implantation, possess unique characteristics such as chemical composition and strong mechanical properties that make them ideal for applications in dentistry and orthopedics.

***Keywords:*** Biomolecules, Bio ceramic, [Drug delivery](https://www.benthamdirect.com/search?value1=%22drug+delivery%22&option1=pub_keyword), Nanomaterial

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**Comparison of the effects of aspirin and salicylic acid on the structural changes and fibrillation of hemoglobin**

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**Abstract**

Hemoglobin is one of the vital proteins in the body, playing a critical role in oxygen transport.​ Aspirin is a widely used medication. Salicylic acid is a natural compound found in various plants, particularly in willow bark extract. On the other hand, aspirin is a synthetic derivative of salicylic acid. Current research investigates and compares the effects of aspirin and salicylic acid on the structural changes and fibrillation of human hemoglobin. The methodology employed in this experimental study was investigated using spectroscopic techniques, including circular dichroism (CD), intrinsic fluorescence spectroscopy, and scanning electron microscopy (SEM). The results obtained from the intrinsic fluorescence emission through the incubation method indicate that the position of heme prosthetic group in hemoglobin-aspirin has changed or caused heme degradation more than hemoglobin-salicylic acid compared to the initial state.​ Findings from the circular dichroism spectroscopy, which was examined via the incubation approach, revealed a more significant alteration in the secondary structure of hemoglobin incubated with different concentrations of aspirin compared to salicylic acid. Additionally, the results from scanning electron microscopy (SEM) demonstrated that the sample incubated with aspirin exhibited a greater number and larger size of fibrils compared to the sample incubated with salicylic acid.

***Keywords:*** Salicylic acid, Aspirin, Human hemoglobin, Heme degradation, Fibrillation

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**The impact of various organic solvents on the solubility of polyester compounds**

Yasamin Janati, Arastoo Badoei-Dalfard\*, Zahra Karami

**Abstract**

Plastics are organic polymers created through the polymerization of long hydrocarbon chains. Because of their high durability, plastics persist in the environment for a long time. One effective method to break them down and convert them into simpler materials is to use a suitable solvent that alters their structure. Some solvents can break down the structure of a plastic, while others may soften or distort it. The type of plastic and contact time with the solvent also matter. In this study Dimethylformamide (DMF), Dimethyl sulfoxide (DMSO), Phenol, Trifluoroacetic acid (TFA), Dichloromethane, Chloroform, and Toluene were utilized in quantities of 2 ml to assess dissolution rate of small pieces obtained from plastic bottles, which are considered as a source of polyester plastics. Furthermore, constant stirring, boiling the solvent, and the application of heat and time were found to be able to enhance solubility. Results showed that polyester polymers can be transformed from solid to liquid when they’re exposed to suitable solvents. Trifluoroacetic acid (TFA) is the most effective one, able to depolymerize bottles by 50% and dissolve films due to its acidic nature, particularly at high temperatures. Chloroform has 40% solubility, while Toluene has a lower solubility. Phenol and Dimethyl sulfoxide (DMSO) each have 20% solubility, Dichloromethane and Dimethylformamide (DMF) have 10%. Based on our results, Trifluoroacetic acid can be used as the best solvent for polyester degradation.

***Keywords****:* Organic solvents, Solubility, Polyester, Plastics

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**Investigation of chrysin as interleukin 6 potential inhibitor by *in- silico* method**

Tooba Abdizadeh

**Abstract**

Rheumatoid arthritis (RA) is a chronic inflammatory autoimmune disease distinguished by painful inflammation of the joints. Cytokines such as Interleukin 6 (IL-6) have a crucial role in the initiation and development of rheumatoid inflammation. IL-6 is a multifunctional cytokine essential for hematopoiesis, immunology, bone metabolism, and inflammation. This study aimed to investigate the molecular mechanism of chrysin in the treatment of rheumatoid arthritis using a molecular docking approach. Molecular docking studies were performed using Autodock software. The 3D structure of the chrysin was obtained from PubchemPubChem and converted into PDB format by AutoDock software for docking analysis. Afterward, the IL-6 protein was taken from the Protein Data Bank (PDB), and molecular docking was done with chrysin by using the Autodock software. Then, the obtained results were analyzed by Chimera software. Molecular docking has shown high binding affinity for the chrysin to IL-6 protein. The ligands interacted with IL-6 residues in the active site of the protein, which may be important for IL-6 inhibitory activity. This study can provide evidence to consider chrysin as a natural product with further research in vitro and in vivo in the treatment of rheumatoid arthritis.

***Keywords:*** Rheumatoid arthritis, Chrysin, Molecular docking

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**Green synthesis of magnetite Fe3O4 nanoparticles and biomedical applications in intelligent drug delivery system**

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**Abstract**

Nanotechnology has gained much attention for its potential application in medical science. One intelligent delivery technique that has gained prominence in recent years is the use of magnetic nanoparticles magnetic nanoparticles have demonstrated a promising effect in various biomedical applications. Fe3O4 magnetic nanoparticles are widely applied due to their superparamagnetic properties, high biocompatibility, non–toxicity, large–scale production, recyclability, chemical stability, innocuousness. Magnetic Nanoparticles have been employed in various biomedical applications as drug delivery, magnetic resonance imaging (MRI), cell tracking, gene therapy, tissue engineering and stem cells tracking.Various factors control the magnetic properties of Iron oxide nanoparticles such as shape, size, crystal structure and particle size distribution.Usually Drugs are attached to the surface of magnetic nanoparticles or encapsulated within a nanocomposite mixture of a polymer and magnetic nanoparticle. The intelligent release of drugs to the damaged tissues of the body is one of the most important aspects of the drug delivery system. In intelligent drug delivery system, drug loaded Fe3O4-NPs can accumulate at the site by the aid of external magnetic field. Drug loaded nanoparticles should release the drug at the targeted site at an appropriate rate without harming the healthy cells. In order to apply Fe3O4-NPs in human body, Fe3O4-NPs have to be biocompatible and biodegradable to minimize the toxicity. So, green synthesis plays a crucial. Many researches showed the promising results of Fe3O4-NPs in treating Damaged cells via in- vitro study. Therefore, Fe3O4 nanoparticles are suitable for intelligent drug delivery.

***Keywords:*** Magnetic nanoparticles, Drug delivery, Nanocarrier, Biomedicine

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**Computational approaches to accelerate drug discovery**

Roghayeh Heiran\*

**Abstract**

Protein-ligand interactions are fundamental to numerous biological processes. These interactions are indispensable for cellular communication, metabolic pathways, immune responses, and numerous other vital functions. A comprehensive understanding of protein-ligand interactions is crucial for drug discovery and development. This study examines the intricate mechanisms underlying these interactions, with a focus on the role of non-covalent forces such as hydrogen bonding, electrostatic interactions, van der Waals forces, and hydrophobic effects. By elucidating the molecular determinants of binding affinity and specificity, various drug design strategies have been explored to target specific proteins implicated in disease pathogenesis. This involves understanding the intricate interplay of non-covalent interactions, including hydrogen bonding, electrostatic interactions, van der Waals forces, and hydrophobic effects, that govern the formation of protein-ligand complexes. Computational approaches, such as molecular docking and dynamics simulations, have become indispensable tools in drug discovery, enabling the identification of novel protein targets, pharmacophore mapping, molecular docking, virtual screening of lead compounds, prediction of bioactivity, simulation of protein-ligand complex dynamics, affinity prediction, and the design of optimized ligands. These techniques enable researchers to virtually screen vast chemical libraries, identify potential drug candidates, and refine their structures to enhance binding affinity and selectivity. By simulating the dynamic behavior of protein-ligand complexes, these computational methods provide valuable insights into the molecular mechanisms underlying drug action, ultimately accelerating the drug discovery process.

***Keywords:*** Protein-ligand interaction, Molecular docking, Dynamics simulations, Drug discovery

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**Preparation of exfoliated MoS2 nanosheets with catalytic active edges**

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**Abstract**

Two-dimensional MoS2 nanosheets have been widely studied in diverse application fields (1). MoS2 nanosheets can be prepared via different synthesis methods such as hydrothermal/solvothermal and liquid-phase-exfoliation method ~~(2).~~ In this study, MoS2 nanosheets have been prepared through exfoliation of bulk MoS2 powder in N-methyl-2-pyrrolidone (NMP) via combination of bath and then tip sonication. In order to activate the MoS2 nanosheets edges, appropriate amount of highly oxidant H2O2 was added to NMP solution. The best results were obtained where the volume ration of 3:17 (V/V%) was chosen for H2O2: NMP. Obtaining catalytic active MoS2 nanosheets via such a facile and straightforward procedure is an important achievement for various applications such as water splitting and pollutants degradation ~~(3).~~

***Keywords:*** MoS2, H2O2, NMP, Exfoliation

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**Study of the effect of tramadol on serum biochemical parameters in male Wistar rats**

Dariush Gholamia,\*, Seyed Hossein khaleghinezhadb

**Abstract**

Nowadays, the use of pain-controlling drugs in various surgeries is common. One of these drugs is tramadol. Tramadol is a synthetic opioid with central activity. In this study, the effects of this drug on the activity of liver enzymes, blood urea nitrogen (BUN), and creatinine in mice were investigated. For this purpose, 15 male Wistar rats were used and divided into three equal groups (control group, group receiving tramadol hydrochloride at a dose of 2 mg/kg, group receiving tramadol hydrochloride at a dose of 5 mg/kg). The present study showed that acute and chronic administration of tramadol had a significant effect on serum biochemical and hematological parameters in male Wistar rats. Therefore, it is recommended to be more cautious in using this drug to relieve pain in patients undergoing treatment and surgery.

***Keywords:*** Tramadol, Blood parameters, Biochemical parameters, Male rats

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**Eco-friendly synthesis of zinc oxide nanoparticles using Ficus religiosa leaves**

Fatemeh Sedaghatia,\*, Mahdieh Kheyrib, Fayezeh Samarib,c

**Abstract**

Green synthesis represents an innovative approach to nanomaterial production, leveraging biological entities such as plants, fungi, and algae as reducing and capping agents. This sustainable methodology offers a compelling alternative to conventional chemical methods, which often rely on toxic chemicals and generate harmful byproducts [1]. Ficus religiosa, commonly known as the sacred fig or peepal tree, has emerged as a promising natural resource for the green synthesis of nanoparticles.

This study presents a novel and green method for synthesizing zinc oxide nanoparticles (ZnO NPs) utilizing Ficus religiosa leaf extract as a renewable, non-toxic, and effective stabilizer. Optimizing the synthesis process to achieve specific nanoparticle properties, including size, shape, and crystallinity, is of significant importance. The amount of leaf extract, temperature, and reaction time are crucial parameters that significantly influence the synthesis process and subsequent properties of the nanoparticles.

The quantity of leaf extract and calcination temperature were optimized and the volume of leaf extract=60 ml and T=400 ⸰C were considered. Along with the synthesis and fabrication processes, it is necessary to characterize nanoparticles to assess their properties, so, information on the size, morphology, chemical composition, crystal structure, surface composition, optical band-gap value, and thermal stability were concluded using some of the most common characterization techniques.The results confirmed the successful synthesis of ZnO nanoparticles, which exhibited a spherical morphology with an average size of 50 nm and a band gap energy of 3.14 eV.

***Keywords:*** Green synthesis, Zinc oxide nanoparticles, *Ficus religiosa*, Leaf extract

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**An investigation towards MIL-101 (Fe-Cu) structures to achieve optimal activity across a pH range**

Aida Davaria, Arastoo Badoei-Dalfarda,\*, Zahra Karamia, Shahriar Dabirib

**Abstract**

Metal-organic frameworks (MOFs) are compounds consisting of metal and organic linkers with properties such as high porosity, chemical and thermal stability, and structure tunability that have diverse applications including catalysis, biosensors, and drug delivery in the fields of industry, therapy, and medicine. Due to combination of nanozyme and enzyme in biosensing fields to measure metabolites, pH is one of the most effective factors related to functional performance of both nanozyme and enzyme, so it should be optimized. In this study, the bimetallic structure MIL-101 (Fe/Cu) was prepared with different Iron to Copper ratios (5:1, 2:1, 1:1, 1:2, and 1:5) and its Peroxidase-like activity was investigated in the pH range of 4 to 6.5. The results showed that the optimal pH is about 4.5, but the ratio of metals plays a key role in increasing the catalytic activity at other pHs. The compounds (Fe:Cu 1:2) and (Fe:Cu 1:5) compounds had a relatively rapid decrease in activity with increasing pH, like compound (Fe:Cu 5:1), although their absorption level at pH 4 was more than 2 times the value reported for (Fe:Cu 5:1). These findings indicate that designing and tuning the metal ratio in bimetallic MOFs can improve their catalytic efficiency in biosensing applications.

***Keywords:***  Metal Organic Frameworks, Nanozyme, Peroxidase, Fe-Cu, Activity

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**Simulating the release of metformin as anti-diabetic drug from carbon nanotubes**

Fateme Malayjerdia, Nasrin Mollaniaa, Mohsen Abbaspourb, Rasoul Esmaeely Neisianyc,d, Ali Ashtariyanc

**Abstract**

Diabetes mellitus (DM) and its complications constitute a serious public health issue facing modern societies (1). Metformin is currently the most widely used hypoglycemic drug for diabetes mellitus (2). Furthermore, in recent years, it has been determined that, this drug has direct effects on cancer cells.

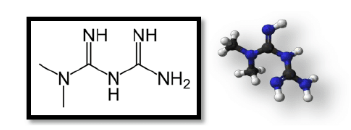


Fig. 1: Structure of N'N-Dimethylimidodicarbonimidicdiamide (Metformin

Based on previous research, it was demonstrated that metformin loaded on carbon nanotubes under near-infrared (NIR) irradiation led to a significantly increased response to cancerous cells. Molecular dynamics simulations are a very powerful method to Study the drug delivery process and improve its efficacy and safety by controlling the rate, time, and place of release of drugs. in this study the dynamic release of metformin from the interior of carbon nanotube in the aquatic environment using the dl-poly software.

***Keywords:*** Diabetes, Diabetes mellitus, Metformin, Molecular dynamics simulation

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**Antibacterial agents: Design and *in- silico* studies**

Roghayeh Heirana,\*, Elham Riazimontazerb,c,d

**Abstract**

The emergence of antibiotic resistance poses a severe threat to global health. β-lactams, a class of antimicrobial agents renowned for their broad-spectrum activity, favorable pharmacokinetic properties, low toxicity, oral bioavailability, and bactericidal action, have been a cornerstone of antimicrobial therapy. These agents exert their antibacterial effect by inhibiting the catalytic activity of bacterial transpeptidases, also known as penicillin-binding proteins (PBPs), which are essential enzymes in the cross-linking of peptidoglycan chains during cell wall synthesis. In this study, we designed a series of monocyclic β-lactams incorporating diverse substituents. These compounds were subsequently evaluated for their inhibitory potential against PBP, a crucial target in bacterial cell wall biosynthesis, using molecular docking simulations with the validated PDB structure 1MWT. Visual analysis of the docking results revealed favorable interactions between the designed compounds and the active site residues of PBP. Notably, several compounds exhibited promising binding affinities and could potentially serve as lead candidates for the development of novel antimicrobial agents to combat infectious diseases.

***Keywords:*** 2-Azetidinone, Molecular docking, Antibacterial, Drug design

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**Biosynthesis of iron oxide nanoparticles by *Bacillus sp.* GFCr-1**

Fahimeh Mollania, Fariba Mollaniaa, Nasrin Mollaniab

**Abstract**

Nanostructured materials, including iron oxide nanoparticles (IONPs), have important application in nanotechnology due to their unique properties (1). Various studies have been conducted to biosynthesize these nanoparticles using extremophile bacteria (2, 3). The aim of this study was to optimize iron oxide nanoparticle biosynthesis by Bacillus sp. GFCr-1 in the invitro condition. The biosynthesized IONP was characterized by UV-vis spectrophotometry at 370 nm, X-ray Diffraction (XRD), and scanning electron microscope (SEM). In the first, changing the medium reaction color to dark brown indicated the biosynthesis of iron oxide nanoparticles.

***Keywords:*** Biosynthesis, Iron oxide nanoparticles, Bacillus sp

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**Stability of encapsulated glucose oxidase in polyacrylamide gel**

Bahareh Farahani Mehrabi, Leila Hassani\*

**Abstract**

Glucose oxidase is an important enzyme has extensively used in industry and medicine, so stabilization of this enzyme is of great importance in biotechnology. Environmental conditions like temperature, organic solvents and pH have influence on the enzyme stability. There are several strategies like immobilization, protein and solvent engineering to increase stability of enzymes and maintain their structure during storage and application. In this research, glucose oxidase was encapsulated in polyacrylamide gel as an immobilization method and its stability was evaluated by absorption spectroscopic technique. For encapsulation, N-acryloxysuccinimide (NAS) as linker that binds to lysine residue was added to the enzyme solution and then the enzyme was encapsulated in the gel by adding acrylamide and bisacrylamide. Various encapsulated samples were prepared at different concentrations of the linker and acrylamide. The remaining activity of the enzyme at 50oC was measured and the results indicated that at the low ratio of linker and the gel material to the enzyme, encapsulation has no remarkable effect on the protein stability, but at the high ratio, stability of the enzyme decreases to some extent. Stability of the enzyme at 40% and 50% DMSO organic solvent indicated that the encapsulation not only in the low concentration, but also at the high concentration of the gel has no meaningful effect on the enzyme stability. Consequently, encapsulating condition that leads to tight or lose encapsulation influences on the enzyme stability and finding the optimum condition for encapsulation is an important factor for stabilization of the enzyme through encapsulation.

***Keywords:*** Stabilization, Glucose oxidase, Polyacrylamide gel, Encapsulation

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**Protein replacement therapies for recessive Dystrophic epidermolysis bullosa (RDEB)**

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**Abstract**

Recessive dystrophic epidermolysis bullosa (RDEB) is a debilitating genetic disorder caused by mutations in the COL7A1 gene encoding type VII collagen (C7), an essential component of the dermal-epidermal junction (DEJ). This deficiency results in extreme skin fragility, blistering, and chronic wounds, significantly impairing patients’ quality of life and increasing the risk of skin cancer (1, 2). Recent advancements in protein replacement therapy have shown promise in addressing the underlying cause of RDEB by restoring C7 function. Studies in murine models lacking C7 have demonstrated that intravenous and topical administration of recombinant human C7 (rhC7) can effectively incorporate into the DEJ, leading to the reformation of anchoring fibrils and improved skin integrity (3). This approach reduces skin fragility and blistering, ultimately extending the survival of affected animals. The potential of rhC7 to serve as a therapeutic agent for RDEB is further bolstered by its ability to evade significant immune responses, particularly when mechanisms like the CD40-CD40L pathway are inhibited to prevent antibody generation (2, 4). The half-life of C7 in the DEJ is approximately 30 days, necessitating considerations for dosage and frequency to maintain therapeutic levels in human applications (5). Innovations in recombinant technologies have facilitated the production of stable, disulfide-bonded C7 trimers that form effective dermal-epidermal anchors, even in pathogenic mutations (6). Such mutations, while posing challenges due to the potential for protein misfolding or increased proteolytic sensitivity, underscore the importance of tailoring protein therapy to individual genetic profiles (6). Furthermore, topical applications of recombinant C7 in mouse models have demonstrated efficacy in promoting wound closure and minimizing scar formation by modulating transforming growth factors, suggesting additional therapeutic pathways for chronic wound management beyond genetic correction (7). This indicates a dual potential for C7 therapies to restore structural integrity and enhance regenerative healing processes, emphasizing the need for comprehensive approaches that integrate gene, protein, and immune modulation strategies in treating RDEB (8, 9). Complementing direct protein therapies, biomaterial advancements such as RHC-conjugated chitosan hydrogels offer innovative solutions for wound management. These hydrogels, incorporating recombinant human collagen-peptide (RHC), support enhanced mechanical properties and bioactivity, addressing the typical limitations of traditional chitosan hydrogels (10). The thermosensitive properties of such hydrogels enable better handling and application flexibility, which is critical for treating complex wounds like burns.

In- vitro and in vivo studies reveal that RHC-chitosan hydrogels significantly promote cell viability, infiltration, and vascularization, which are crucial for tissue regeneration and repair (10). The hydrogel matrix provides a supportive environment that facilitates cell migration and integration, which, paired with increased mechanical stiffness and optimized water vapor transmission, accelerates the healing process and improves clinical outcomes (10). This dual focus on structural and therapeutic attributes highlights the promising future of combined cell-based, protein, and biomaterial therapies for RDEB and other conditions characterized by structural protein defects. Continued research and clinical evaluation will be vital to refine these techniques and verify efficacy and safety in human populations, potentially transforming treatment paradigms for genetic skin disorders (1, 10). In summary, the convergence of protein replacement therapies and advanced biomaterials like RHC-conjugated hydrogels represents a significant leap forward in treating severe dermatological conditions. These emerging strategies provide a foundation for innovative, personalized therapeutic interventions that may soon extend beyond the scope of RDEB to tackle a range of complex wound healing challenges (2, 9, 11).

***Keywords:*** Recessive Dystrophic Epidermolysis Bullosa (RDEB), Protein replacement therapy, Recombinant biomaterials, Chitosan hydrogels

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**Molecular dynamics and bioinformatics investigation of spike protein mutations in SARS-CoV-2 from the Wuhan strain to the XEC variant**

Yahya Sefidbakht

**Abstract**

Since its emergence, SARS-CoV-2 has undergone significant evolutionary changes, particularly in the spike protein, resulting in the emergence of variants of concern (VOCs) such as Alpha, Beta, Gamma, Delta, and Omicron. Mutations in this protein have enhanced viral transmissibility, ACE2 receptor binding affinity, immune evasion, and pathogenicity, facilitating the global spread of new variants. This study aims to investigate the effects of recent mutations on the structure and dynamics of the SARS-CoV-2 spike protein using molecular dynamics (MD) simulations. Furthermore, the influence of these mutations on the spike protein’s interactions with the ACE2 receptor and its antigenic properties is analysed and evaluated. MD simulations were conducted for the wild-type and mutant spike proteins in complex with the ACE2 receptor using GROMACS (version 2020.6). The CHARMM36 force field was employed for system parameterization, and each system was simulated for 100 nanoseconds. Structural stability, binding free energy, and conformational changes were analyzed to assess the impact of the mutations. Preliminary analyses indicate that certain mutations enhance the spike protein's binding affinity to ACE2 by stabilizing critical interface regions, while others facilitate immune evasion through alterations of surface-exposed epitopes. Dynamic analyses reveal changes in flexibility, stability, and structural dynamics, which are predicted to contribute to increased viral pathogenicity. Specifically, the XEC variant, a recombinant of KS.1.1 and KP.3.3, benefits from the rare T22N mutation (from KS.1.1) combined with Q493E (from KP.3.3), enhancing immune evasion and receptor binding. The findings of this study provide a detailed molecular understanding of how spike protein mutations drive the emergence and spread of new SARS-CoV-2 variants. Therefore, this could enhance vaccine design and inform therapeutic strategies to combat future variants.

***Keywords:*** SARS-CoV-2, Spike protein, Molecular dynamics, Variants of concern, Immune evasion

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**Stabilization of photoprotein aequorin through mutagenesis and Deep eutectic solvents**

Zahra nava, Reza H. Sajedi\*

**Abstract**

Aequorin, a calcium-regulated photoprotein, has diverse applications in biosensing and imaging [1-2]. However, its stability limits its broader usage, particularly under harsh conditions [3]. This study investigates the impact of two types of deep eutectic solvents (DES), choline chloride-glycerol (ChCl-Gly) and choline chloride-urea (ChCl-Urea), on enhancing of structural and thermal stability of G14A mutant of aequorin. so far, there has been a steady increase in utilization of these solvents on protein stabilization [4]. The G14A mutation, because of local increase in the number of van der Waals interactions, is hypothesized to influence its stability and folding properties [5]. The G14A variant of aequorin was expressed in *E. coli* BL21(DE3) cells and purified using affinity chromatography. Structural analysis was performed using Far-UV circular dichroism (CD) spectroscopy, while intrinsic fluorescence measurements and thermal stability assays were employed to assess the protein's structural integrity and heat tolerance in the presence of DESs. The stability of G14A aequorin was evaluated by monitoring changes in secondary structure and fluorescence intensity after exposure to DES solutions at different time intervals (5, 10, 15, 30, and 60 minutes) at 70 °C. Far-UV CD spectra revealed that both ChCl-Gly and ChCl-Urea significantly increased the secondary structure content of G14A aequorin compared to the control. The intrinsic fluorescence intensity of this mutant in the presence of ChCl-Gly was significantly decreased compared to the control, while ChCl-Urea caused a minor increase in emission. Thermal stability assays showed that G14A in the presence of both ChCl-Gly and ChCl-Urea buffers exhibited improved stability over time at 70 °C. Both DES buffers facilitated increased protein stability compared to the control, indicating a protective effect on the protein’s conformation. The G14A mutation, in combination with DES buffers, enhances the stability of aequorin, making it more robust and applicable for a broader range of biotechnological and analytical applications.

***Keywords:*** Aequorin, Deep eutectic solvents, Choline chloride-glycerol, Choline chloride-urea

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**Evaluation the origin of conformational and tautomeric preferences in N-acetylacetamide- a quantum chemical study**

Mahdiye Poorsargoa,\*, Fatemeh Rigib

**Abstract**

Quantum chemical study of N-acetyl acetamide was carried out at various theoretical levels such as HF, B3LYP and MP2 methods with the most popular basis set, 6-311++G (d, p). The computational results reveal that the amide resonance and intramolecular hydrogen bonding are two superior factors in determining the most stable conformation of diamide and amide–imidic acid tautomers, respectively. The evaluation of hydrogen bond energies predicts that the hydrogen bond strength of N-acetyl acetamide is weaker than acetyl acetamide. But the results of atoms in molecules, natural bond orbital, and geometrical parameters are given a different order, EHB (N-acetyl acetamide) > EHB (acetyl acetamide). Although the bond average energies of tautomerization process emphasized on more stability of amide–imidic acid tautomer, but our theoretical calculations reveal that the diamide conformers are more stable than the amide–imidic ones. The population analyses of equilibrium conformations by natural bond orbital method also predict that the origin of tautomeric preference is mainly because of the electron delocalization of amide functional group, especially LP(N)→ π\*C=O charge transfer.

***Keywords:*** N-acetyl acetamide, Intramolecular hydrogen bond, Amide resonance, AIM, NBO

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**Theoretical study of the adsorption of anticancer drug ibrutinib on the boron nitride single-walled nanotubes**

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**Abstract**

New drug delivery in cancer treatment is a strategy to reduce the side effects of chemotherapy. Different types of carriers are used for drug delivery. Among these carriers are boron nitride nanotubes. In this research, single-walled boron nitride nanotubes were investigated as carriers of anticancer drug, ibrutinib. The absorption of this drug was investigated in two positions inside and outside boron nitride nanotubes with different diameters. Based on the Lennard-Jones energy values between drug and nanotube and RDF curves, drug absorption in both positions are thermodynamically favorable. The simulation results showed that the interaction between the drug and the nanotube in the inner position is stronger than the outer position. The diameter of nanotubes had an effect on the interaction energy between nanotubes and drug. The strongest interaction between ibrutinib was related to the internal position of the BN nanotube (9, 9) with a diameter of 12.20 A. It was also observed that the strength of interactions between nanotubes and drug in the inner position decreases with the increase in diameter of nanotubes, but the strength of interactions between nanotubes and drug in the outer position does not change much with the increase in diameter of nanotubes. The strong interaction of drug absorbed on the outer surface of nanotubes with water molecules improves the solubility of nanotubes.

***Keywords:*** Anti-cancer drug, Ibrutinib, Adsorption, Boron-nitride nanotubes

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**Enhanced D-HPG synthesis using Surface-displayed enzymes in E. coli**

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**Abstract**

D-p-Hydroxyphenylglycine (D-HPG) is an essential building block for the synthesis of semisynthetic antibiotics, such as amoxicillin and cefadroxil. Traditionally, D-HPG is produced through chemical synthesis, which involves harsh reaction conditions, high energy consumption, and generates significant environmental waste [1,2]. While enzymatic production offers a greener alternative, conventional approaches require the purification of the two key enzymes involved, D-hydantoinase (D-Hase) and D-carbamoylase (D-Case), before use. This purification step is labor-intensive, costly, and time-consuming, limiting the practicality of enzymatic methods. The surface display system, which anchors enzymes directly to the surface of the cell, addresses this limitation by bypassing the need for enzyme purification. [3-5]. In this study, we employed a surface display system on *E. coli* BL21(DE3) to produce D-HPG efficiently. D-Hase hydrolyzes hydantoin derivatives to N-carbamoyl-D-amino acids, which are further converted to D-amino acids by D-Case. We constructed recombinant *E. coli* BL21(DE3) strains with surface-displayed D-Hase and D-Case by designing fusion constructs for efficient enzyme localization. Expression conditions were optimized to enhance enzyme activity. Semi-quantitative enzymatic activity analysis using Ehrlich’s reagent confirmed the functionality of the surface-displayed enzymes. D-HPG production was analyzed using thin-layer chromatography (TLC) and high-performance liquid chromatography (HPLC). Quantitative HPLC measurements demonstrated a high production yield of approximately 95%. This method offers significant advantages over traditional approaches, including mild reaction conditions, reduced environmental impact, and cost-effectiveness. In conclusion, this study highlights the successful application of a surface display system on *E. coli* for whole-cell biocatalysis of D-HPG. This innovative method provides a sustainable and efficient alternative to traditional chemical synthesis, offering great potential for industrial-scale production of D-HPG.

***Keywords:*** Bacterial surface display, D-p-hydroxyphenyl glycine, D-hydantoinase, D-decarbamoylase

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**Investigating the expression of recombinant protein of survivin in BL21 and C41 bacterial strains**

Mahsa Tirmomenin, Farangis Ataei\*, Saman Hosseinkhani

**Abstract**

One of the precise methods for producing recombinant proteins is expression in bacteria. In the last decade, producing these types of proteins has made significant progress in industry. The gram-negative bacteria Escherichia coli is known due to factors such as having an easy and cheap culture medium, short life cycle, and rapid growth and genetic expression. The main problem of this expression system is the production of non-functional proteins in the form of inclusion bodies, which unlike mammals, do not have organizations to achieve folding and post-translational motifs. To solve this problem, scientists often use methods such as changing the vector / changing the parameters of the culture medium from the recombinant host strain / changing the host, etc., to express and produce proteins at high levels. Our study focuses explicitly on survivin, the smallest protein member of the apoptosis inhibitor family. Survivin has been found in both the cytosol and mitochondria, which it is called a nuclear export signal, and it is also known as a tumor marker. Our study investigates the expression of recombinant protein (survivin) in BL21-and C41 expressing bacteria. We are particularly interested in the presence of two type inducers and comparing the expression of two bacterial strains from Escherichia coli BL21 and C41. This comparison is crucial to our research and provides valuable insights into survivin expression. The pET-28a vector containing the wild-type survivin gene was transformed to *Escherichia coli BL21* expression and C41, separately. The expression of recombinant protein was induced with 0.5 mM IPTG and/or 4 mM lactose at the different times and temperatures (37, 30, 22, and 18 °C), in a shaker incubator. The protein expression levels were checked by 17.5% SDS PAGE gel. Under all conditions, BL21-expressing bacteria produced protein in a significant amount of soluble form. Also, the expression of recombinant protein in the presence of IPTG inducer was greater than that of lactose as insoluble form. Also, the results showed that the expression in C41 bacteria is less than in BL21 bacteria, but higher level of protein was observed in soluble form in supernatant of lysed bacteria. This research contributed to optimizing expression parameters.

***Keywords:*** Survivin, Expression, BL21-C41 bacteria*,* IPTG, Lactose

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**Cloning, expression, and characterization of a novel marine L-asparaginase from *Pseudomonas aeruginosa HR03***

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**Abstract**

The present study focused on the cloning, expression, and characterization of marine L-asparaginase of *Pseudomonas aeruginosa HR03* isolated from fish intestine (*L.klunzingeri*). Marine *Pseudomonas aeruginosa HR03* was used for retrieving the l-asparaginase encoding gene (HR03Asnase) of size 936 bp. The gene was successfully cloned into the pET21a vector and expressed into *Escherichia coli BL21* (DE3) for characterization of the protein. The recombinant HR03Asnase enzyme was purified by affinity chromatography using nickel affinity chromatography, and the enzymatic properties of HR03Asnase, including the effects of pH and temperature on HR03Asnase activity and kinetic parameters, were determined. The recombinant enzyme HR03Asnase showed the highest similarity to type I bacterial L-asparaginase from *Pseudomonas aeruginosa*. The three-dimensional (3D) modeling results indicate that HR03Asnase exists as a homotetramer. Also, The Molecular weight analysis using SDS-PAGE revealed ~ 35 kDa. The HR03Asnase showed optimum pH and temperature of 8.0 and 40 °C, respectively. The maximum activity of HR03Asnase was reduced by 50% at 90 °C after 10-min incubation; though, the enzyme preserved more than 20% of its activity after 30-min incubation. This enzyme also preserved almost 50% of its activity at pH 12 after 40-min incubation. The km and Vmax of the enzyme obtained with l-asparagine as substrate were 10.904 mM and 3.44 × 10−2 mM/min, respectively. The recombinant HR03Asnase of marine *P. aeruginosa* may also be explored as a potential agent in pharmaceutical and food applications. The assessment of pH and temperature stability of HR03Asnase showed that the enzyme has a wide range of activity, which is a suitable characteristic for its application in different industries. Overall, the results of the present study show that marine sources are promising biological reservoirs for enzymes to be used for biotechnological purposes, and marine thermostable HR03Asnase is likely a potential candidate for its future usage in the pharmaceutical and food industries.

***Keywords:*** Purification, Cloning, E. coli, Enzyme activity, Acrylamide

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**Advancing Alzheimer's disease research and drug discovery through the use of artificial intelligence**

Mohammd Hossein Ebrahim Abadia, Ali-Reza Manavi Amina, Yahya Sefidbakhta,\*, Maryam Haghshenasb, Moslem Afrashtehc, Sina Mozaffari-Jovind, Vladimir N. Uverskye

**Abstract**

Artificial intelligence (AI) and machine learning (ML) have revolutionized Alzheimer's disease (AD) research, driving advancements in both diagnosis and drug discovery. AI-based models, such as convolutional neural networks (CNNs) and support vector regression (SVR), have demonstrated high precision in differentiating between AD, mild cognitive impairment (MCI), and healthy individuals through neuroimaging techniques like MRI and PET. These technologies have enhanced the detection of early AD biomarkers, aiding in more accurate diagnosis. In drug discovery, AI-driven methods like machine learning and deep learning are transforming key processes such as virtual screening, de novo drug design, and pharmacokinetic/pharmacodynamic (PK/PD) modeling. AI plays a crucial role in predicting drug properties related to absorption, distribution, metabolism, excretion, and toxicity (ADMET), particularly in evaluating blood-brain barrier (BBB) penetration. Models like support vector machines (SVM) and light gradient boosting machine (LightGBM) have achieved high accuracy in predicting BBB permeability, accelerating the development of therapeutic candidates. Furthermore, AI integration in multi-omic data analysis, utilizing public datasets like ADNI and NIAGADS, has enabled the identification of key genes and pathways involved in AD, which serve as potential drug targets. Advanced machine learning techniques, including logistic ridge regression, random forest, and support vector machines, have identified critical pathways like mitochondrial dysfunction and NF-kappa B signaling in AD pathogenesis. Overall, AI has been pivotal in AD research, improving early diagnosis and expediting drug discovery, offering promising avenues for future treatments and precision medicine.

***Keywords:*** Artificial intelligence, Alzheimer's disease, Drug discovery, Multi-omics analyses, Machine learning

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**Synthesis, characterization, and interaction studies of a novel Schiff-Base ligand with Human Serum Albumin (HSA): Spectroscopic and molecular docking investigation**

Farzad Hosseinia, Ahmad Amirib,\*

**Abstract**

Schiff bases and their metal complexes are significant compounds in the medicinal and pharmaceutical fields. Their biological applications have gained traction due to their demonstrated antimicrobial, antifungal, antibacterial, antiviral, antipyretic, antidiabetic, and antitumor properties. Given their potential as anticancer agents, understanding how Schiff bases interact with Human Serum Albumin (HSA), the most prevalent plasma carrier protein, is of great interest. This can be explored through various spectroscopic techniques and molecular modeling. HSA has captured the pharmaceutical industry's interest because of its capacity to bind a wide array of metabolites and drugs, which can profoundly influence the pharmacokinetic characteristics of these drugs. In this research, a new Schiff-base ligand (L2) has been synthesized and characterized using UV–Vis and FT-IR spectroscopy. The interaction between this ligand and HSA was investigated through fluorescence spectroscopy and cyclic voltammetry. The binding affinity of the ligand to HSA was assessed under conditions that simulate physiological relevance, utilizing both molecular docking (MD) and experimental methods. The findings indicated that the complex formation between HSA and the ligand led to the quenching of the protein's native fluorescence at 343 nm, which a static binding mechanism can explain.

***Keywords:*** Schiff base, Human serum albumin, Anticancer potential, Cyclic voltammetry, Molecular docking

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**The power of microbial proteins in clinical diagnostics: A metaproteomic approach**

Kaveh Kavousia,\*, Leila Ghanbari-Mamana, Anna Meyfourb

**Abstract**

Metaproteomics, the study of all proteins expressed by a microbial community, is revolutionizing clinical diagnostics by providing a deeper understanding of host-microbiome interactions. Microbial proteins serve as critical indicators of disease, offering insights into complex pathologies that traditional biomarkers often miss. This study explores the potential of gut microbiome metaproteomics for diagnosing paediatric Inflammatory Bowel Disease (IBD), specifically Crohn's Disease (CD) and Ulcerative Colitis (UC). We demonstrate that microbial protein profiles provide superior diagnostic accuracy compared to conventional methods. By applying machine learning algorithms to metaproteomic data, we developed a diagnostic panel capable of distinguishing between CD and UC with high precision. This non-invasive approach offers a promising alternative for diagnosing IBD, particularly in children where current procedures can be challenging. Our findings highlight the broader significance of omics data, particularly microbiome metaproteome, in modern medicine. Metaproteomic analysis not only aids in accurate diagnosis but also paves the way for personalized medicine. By understanding the functional changes within the microbiome, clinicians can tailor treatments and improve patient outcomes. This study underscores the transformative power of metaproteomics in clinical settings, with potential applications extending beyond IBD to various complex diseases.

***Keywords:*** Metaproteomics, Complex Diseases, Diagnostic Biomarkers, Gut Microbiome, Machine Learning

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**Fibrillar proteins and their role in the removal of heavy metal contamination from water sources**

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**Abstract**

Currently, water pollution caused by heavy metals is an important global phenomenon. Lead and cadmium are among the most important heavy elements that enter water sources through various ways such as industrial and agricultural effluents unsanitary burial places and urban and industrial water materials and cause serious harm to human health. Recently the use of economic absorbents has received much attention. This research aims to evaluate the beta-lactoglobulin (BLG)-lactic acid hybrid protein as a membrane filter in removing heavy metals such as lead and cadmium. Beta-lactoglobulin Protein fibers were prepared by incubation of the protein in pH 2 and lactic acid. Then the BLG-lactic-acid hybrid was studied by ultraviolet-visible spectroscopy, Fourier transform infrared (FTIR) spectroscopy, and scanning electron microscopy (SEM). After performing dialysis, the absorption capacity of the hybrid was evaluated by atomic absorption spectroscopy (AAS) using standard solution samples of lead and cadmium heavy metals. The structure of the fibers was observed by SEM. UV-visible absorption and FTIR spectra showed the formation of a fiber-lactic acid hybrid. The results of mass spectrometry showed that the percentage of hybrid efficiency for lead and cadmium metal were 31% and 25%, respectively. According to the results obtained from this research, the beta-lactoglobulin-lactic acid hybrid is a suitable substrate for the absorption of lead and cadmium heavy metals in polluted waters.

***Keywords:*** Beta-Lactoglobulin, Water refinery, Lead, Cadmium, Lactic acid, Membrane filter

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**Discovering Enzybiotics in metagenomes: Innovative enzymes as sustainable alternatives to antibiotics**

Shohreh Ariaeenejad

**Abstract**

The global rise in antibiotic resistance has necessitated the exploration of innovative and sustainable alternatives to traditional antibiotics. This study introduces "Enzybiotics," enzymes derived from metagenomic datasets that target and degrade bacterial cell components such as DNA, polysaccharides, and proteins, as a promising solution. Enzybiotics disrupt bacterial growth and biofilm formation through various mechanisms, such as degradation of cell walls, disruption of DNA replication, and interference with essential metabolic processes[1,2] . Leveraging metagenomics, the study of genetic material from environmental samples allows access to diverse microbial communities[3,4]. These include those from extreme habitats and plant/animal microbiomes, which offer a source of novel enzymes with unique functionalities[5–7]. Advanced bioinformatics pipelines and machine learning techniques enable the efficient mining of metagenomic data, prediction of enzymatic activities, and prioritization of high-potential candidates. Unlike conventional antibiotics, enzybiotics offer versatility and function independently or synergistically to prevent or degrade biofilms. This dual-action capability positions enzymes as robust biocatalysts for applications in food safety, healthcare, agriculture, and environmental sustainability. State-of-the-art biotechnological tools, including protein engineering, domain swapping, and high-throughput DNA sequencing, have enhanced the discovery and optimization of these enzymes. This research not only highlights the immense potential of enzybiotics to revolutionize biotechnological processes but also underscores their critical role in addressing pressing global challenges, such as antibiotic resistance and microbial spoilage. This research demonstrates the potential of enzybiotics as sustainable alternatives to traditional antibiotics. By integrating metagenomics and advanced biotechnological tools, this study paves the way for novel solutions to combat antibiotic resistance and to promote environmental and human health.

***Keywords:*** Metagenomic, Enzybiotics, Biotechnological tools, Antibiotic resistance

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**Construction and characterization of epidermal growth factor-loaded nano system for the skin topical application**

Khosro Khajeha,\*, Mohammadreza Sadeghianb

**Abstract**

Skin is the largest organ in the body that plays a role in the body's immunity, sensation, and protection. Skin can age and damage for a variety of reasons, and there are several ways to slow it down or prevent it. Different cosmetics are used for this purpose in cosmetics. Human growth factors are one of the most effective uses for this purpose. These factors have low absorption through the skin due to their high molecular weight. With the help of nanoparticles, effective drug delivery systems can be designed to increase the absorption and effectiveness of these growth factors. Liposomes are one of the most widely used materials in the healthcare industry and have shown significant benefits. Flexible liposomes that have a surface activator (Edge Activator) in their structure can perform dermal drug delivery in large quantities and with good biocompatibility. The human epidermal growth factor, which is used as an effective factor in skin rejuvenation, was recombinantly expressed in E. coli and then purified by affinity chromatography. Flexible liposomes were synthesized as growth factor nanocarriers by the thin-layer extrusion method. The lipid composition used in this project was egg yolk phosphatidylcholine (EPC) and tween 80 (TW80) with a ratio of 1:31 (EPC: TW80). Synthesized particle size 130 nm, dispersion index less than 0.2, zeta potential -25 mV, spherical morphology, trapping efficiency 72.12%, loading capacity 1.47%, controlled release of the 7-day drug, and good stability in 10 days were reported for these particles. Liposomal nanocarriers containing recombinant human epidermal growth factor were evaluated for function on fibroblast cells and were completely filled in the scratch test after 72 hours. In the MTT test, no toxicity was observed for liposomes in the studied concentrations of liposomes, and liposomes containing growth factor showed a positive effect on the effect of growth factor.

***Keywords:*** Growth factor, Epidermal growth factor, Nano systems, Liposome, Drug delivery

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**Exploring indole ligand interactions with Human Serum Albumin (HSA) via spectroscopy and Molecular Docking techniques**

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**Abstract**

Indoles represent one of the most promising heterocyclic structures, noted for their distinctive properties attributed to the presence of an electron-rich pyrrole component. Heteroannulated indole derivatives have garnered significant interest due to their diverse biological and pharmacological activities [1,2]. This study reports the synthesis and characterization of an Indole ligand using UV–Vis and FT-IR spectroscopy. The interaction between this ligand and human serum albumin (HSA) was explored through fluorescence spectroscopy and cyclic voltammetry. Human serum albumin (HSA) has attracted considerable interest from the pharmaceutical industry owing to its capacity to bind a broad spectrum of metabolites and pharmaceuticals, which can significantly impact the pharmacokinetic profiles of these compounds [3]. Molecular docking and experimental techniques were employed to evaluate the binding affinity of the ligand to HSA under physiologically relevant conditions. The results demonstrated that the formation of a complex between HSA and the ligand resulted in the quenching of the protein's native fluorescence at 358 nm, which can be attributed to a static binding mechanism.

***Keywords:*** Indole, HSA, Anticancer, Interaction, Molecular docking

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**A review of AlphaFold; A method for protein structure prediction**

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**Abstract**

Proteins are regarded as one of the most important biological macromolecules. Identifying their structure will help researchers understand protein’s function and practical applications. In the past, experimental and classical methods such as X-ray crystallography or NMR were used, with advantages and disadvantages. Today, new methods based on artificial intelligence have made a big change in predicting the structure of proteins, an example of which is the method called AlphaFold. Articles related to the present topic were reviewed from databases such as Google Scholar and PubMed from 2019 to 2024. AlphaFold, a method for predicting the structure of proteins in three versions has been introduced to the world. This method, based on deep learning based on convolutional neural networks, processes input data that are often collected from PDB and accurately and quickly predicts the structure of proteins. This method can be widely used in medical, biological, education, industrial and production cases. Different methods are used in protein structure prediction. New methods that are based on artificial intelligence have attracted the attention of researchers because they have high accuracy and speed. However, in order to gain confidence, they need to be measured.

***Keywords:*** Protein, Protein structure prediction, Artificial intelligence, Deep neural network, AlphaFold

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**Development of an Electrochemical Biosensor Using Sulfonic Acid-Modified Magnetic Nanoparticles for Phenolic Compound Detection**

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**Abstract**

An electrochemical biosensor based on tyrosinase (Tyr) was developed to detect the phenolic compounds across medical, environmental, and industrial applications. The biosensor utilized sulfonic acid (SO₃H)-modified magnetic nanoparticles (MNPs) prepared via a hydrothermal synthesis method followed by in-situ surface functionalization. A magnetic carbon paste electrode was fabricated with an optimal graphite-to-paraffin weight ratio. Subsequently, MNP suspension was deposited on the electrode surface, followed by dropping 15 µL of 4 mg/mL Tyr solution. The biosensor was allowed to stabilize for 24 hours before undergoing electrochemical characterization. Cyclic voltammetry (CV) revealed an apparent electron transfer rate constant (kₛ) of 0.011 s⁻¹ and a formal potential (E˚ʹ) of 0.21 V. Differential pulse voltammetry (DPV) demonstrated the biosensor's performance for catecholamine detection. For cafeic acid, the limit of detection (LOD) was 45.4 µM within a linear range of 1–74 µM, with a sensitivity of 1.68 µA·µM⁻¹·cm⁻² and a Michaelis-Menten constant (Km) of 30 µM. For catechol, the LOD was 68 µM in a linear range of 1–107 µM, with a sensitivity of 1.8 µA·µM⁻¹·cm⁻² and Km of 55.3 µM. For L-DOPA, the LOD was 50.6 µM in a linear range of 1–137 µM, with a sensitivity of 0.9 µA·µM⁻¹·cm⁻² and Km of 68.92 µM. The results suggest that incorporating cross-linking agents such as glutaraldehyde to covalent immobilization of the enzyme on the nanoparticles could further enhance the biosensor's kinetic and electrochemical properties, offering improved reliability and sensitivity.

***Keywords*:** Magnetic nanoparticles, Sulfonic acid modification, Polyphenols, and Carbon paste electrode

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**Antiglycation potential of Oregano (*Origanum vulgare*) leaf extract: A natural approach to combat diabetes-related complications**

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**Abstract**

Diabetes mellitus is a chronic disorder of glucose metabolism with serious clinical consequences. The multi-system complications of diabetes include microvascular and macrovascular endpoints. Persistent hyperglycemic state in type 2 diabetes mellitus leads to the initiation and progression of non-enzymatic glycation reaction with proteins, lipids, and nucleic acids, leading to the formation of advanced glycation end-products (AGEs). These compounds are associated with various chronic conditions, including cardiovascular and neurological diseases, as well as aging. The inhibition of glycation has become a significant focus in biomedical research, with natural compounds from medicinal plants showing great potential as therapeutic agents. Oregano (*Origanum vulgare*), a well-known medicinal plant with anti-inflammatory, antimicrobial, and antioxidant properties. This study aimed to evaluate the inhibitory effects of oregano leaf extract on the production of fluorescent end-products in glycated human serum albumin (HSA). HSA was incubated with a high glucose concentration in the presence or absence of oregano leaf extract for 35 days. The obtained results from spectroscopic techniques indicated that oregano extract significantly reduced the formation of AGEs. Furthermore, circular dichroism (CD) analysis demonstrated that the extract modulates the structural alterations of glycated HSA. These findings highlight the critical role of plant-based interventions in mitigating complications associated with diabetes and glycation.

***Keywords:*** Advanced glycation end-products (AGEs), Diabetes, Glycation, Herbal plants, Human serum albumin (HSA), Oregano

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**Novel approach for the high-yield expression and Purification of bio- active LL-37: Implications for biomedical research**

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**Abstract**

LL-37, the sole human cathelicidin, is a multifunctional antimicrobial peptide with potential applications in wound healing due to its chemotactic, endotoxin-neutralizing, and angiogenic properties. Previous recombinant production approaches have typically involved the addition of N-terminal fusion proteins to enhance peptide expression, requiring complex purification processes that diminish yield and increase costs. This study presents the first successful recombinant production of LL-37 in its active form without N-terminal fusions. The LL-37 gene sequence was cloned with a G4S linker and hydroxyapatite binding domain into the pET21a(+) vector and expressed in *E. coli* Shuffle. The recombinant peptide was purified in a single step via affinity chromatography, achieving a yield of 1.02 mg of LL-37 per liter of culture. To evaluate any effects of C-terminal fused sequences on LL-37 activity, a series of assays were conducted. Antimicrobial assays demonstrated reduced activity of the recombinant LL-37 against *E. coli* and *S. aureus* compared to its native counterpart. Enzyme-linked immunosorbent assay (ELISA) revealed that the recombinant peptide binds to lipopolysaccharides (LPS) in a dose-dependent manner (p < 0.05), confirming its endotoxin-neutralizing capabilities. Wound healing potential was assessed using cell scratch assays on human umbilical vein endothelial cells (HuVEC) and human dermal fibroblasts (HDF), showing that recombinant LL-37 (100 ng/mL) significantly enhanced cell migration, achieving an 86% wound repair rate in contrast to 14% in controls after 12 hours (p < 0.05). Additionally, a cell-based ELISA confirmed the binding of recombinant LL-37 to endothelial cell surface receptors in a dose-dependent manner. Importantly, the recombinant LL-37 displayed no cytotoxic effects on HuVEC and fibroblast cells, even at concentrations up to 25 µg/mL. These findings suggest that the recombinant LL-37 can be produced efficiently without fusion tags, retaining its biological activities, and have significant implications for its use in therapeutic applications for wound healing.

***Keywords:*** LL-37 peptide, Antimicrobial peptide, Wound healing, Cost benefit expression and purification

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**Targeted protein modification: A revolutionary approach in neurodegenerative disease therapy**

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**Abstract**

TPM heralds a paradigm shift in the definition of therapeutic strategies against complex diseases, such as neurodegenerative disorders, particularly Parkinson’s disease, Alzheimer’s disease, and Huntington’s disease. Unlike conventional small-molecule inhibitors, TPM uses bifunctional agents to control protein activity or degradation pathways against previously undruggable targets. Novel approaches, including proteolysis-targeting chimeras and autophagy-tethering compounds, represent new modalities for reducing the levels of pathological proteins, such as misfolded or aggregated alpha-synuclein and tau, which are believed to play a central role in the pathogenesis of these disorders. Neurodegenerative diseases are characterized by toxic protein aggregates disrupting cellular homeostasis and contributing to synaptic and neuronal loss(1). TPM strategies exploit either the UPS or autophagy-lysosome pathway for aggregate degradation and, thus, afford a very specific and effective therapeutic intervention. Recent advances have emphasized the potential of bifunctional molecules that selectively bind pathological proteins, thereby tethering them to the cellular degradation machinery and stimulating their removal with minimal impact on normal proteins. Such specificity minimizes off-target effects—a critical limitation of conventional therapies. This review represents recent progress in TPM technologies, highlighting the design of small-molecule ligands capable of inducing protein degradation and stabilization. We review various applications related to the modulation of neurotoxic protein aggregates, attenuation of oxidative stress, and restoration of cellular homeostasis related to neurodegenerative diseases. Modern tools of TPM, integrating ATTECs targeting autophagy pathways with PROTACs inducing ubiquitination of pathogenic proteins, highlight a strong potential for halting disease progression and promoting neuronal function and survival recovery. These results point to the role of TPM as a transformative intervention in the field of neurodegenerative disease treatment, filling critical gaps in current therapies. The development of this area opens unparalleled opportunities for drug discovery and points toward the possibility of personalized and disease-modifying interventions, marking a significant leap in combating such destructive disorders(2).

***Keywords:*** Targeted protein modification, Neurodegenerative diseases, Autophagy, Protein aggregation, Therapeutic innovation

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**Using gold nanoparticles for combination therapy of gemcitabine**

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**Abstract**

The most of chemo drugs have short half-life. The inadequate sustained release can lead to severe side effects, including myelosuppression and nephrotoxicity. In our studies were used the properties of gold nanoparticles (AuNPs). For example, one of them presents a novel nano-drug delivery system utilizing AuNPs optimized with ascorbyl palmitate (AsP) to enhance gemcitabine hydrochloride (GEM) stability and therapeutic efficacy. AuNPs were modified using a single-phase emulsification technique to create a nano emulsion coated with a hydrophobic AsP layer, resulting in improved tumor targeting through the enhanced permeability and retention (EPR) effect. Besides that, in another study AuNPs was synthesized by PEG. The modified AuNPs was immobilized by GEM and Paclitaxel (PAX). The formulations demonstrated a sustained release profile, and enhanced cytotoxicity in the 4T1 and MIA-PACA-2/ PACA-1 cell lines, respectively. Significantly outperforming free GEM/PAX and modified Au-GEM/Au-PEG-GEM/PAX formulations. Notably, for AuNPs-GEM/AsP and Au-PEG-GEM/PAX, those exhibited several months of accelerated stability, attributed to amide bond formation in the functionalized AuNP matrix. The study highlights the synergistic effects of AsP or PAX in enhancing the therapeutic efficacy of Au-GEM-based formulations, supporting its role as a key component in combination therapy. These researches lay the foundations for future developments AuNPs devices that combine chemo drugs for therapeutic and diagnostic applications in nanomedicine.

***Keywords:*** Gold nanoparticles, Combination therapy, Gemcitabine, Paclitaxel

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**Computational study of the complex formation between olive oleuropein and several plant proteins for the purpose of food enrichment**

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**Abstract**

The direct use of natural phenolic compounds in the food industry is usually limited due to their instability and unpleasant taste. Oleuropein is the main phenolic compound in olive leaf, a bioactive compound which has antioxidant and anticancer effects. Encapsulation of bioactive materials can protect them during processing or mask their unpleasant flavor. Among natural biopolymers, plant proteins have many advantages and can be used for various applications, including encapsulation in the food industry. Since wheat, soy and chickpeas are important sources of plant proteins in the human diet; three proteins of chickpea legumin, soy glycinin and wheat agglutinin were selected to study the formation of complexes with oleuropein. In this study, oleuropein was first evaluated for biophysicochemical properties by the SwissADME server. Three-dimensional structure of the proteins was downloaded from the protein data bank and after preparing, the possible binding sites of oleuropein on the proteins were investigated using molecular docking using Auto dock 4.2.6 software. Results showed that oleuropein can bind to legumin, glycine and agglutinin by hydrogen and hydrophobic interactions. Legumin showed four binding sites for oleuropein that the binding free energy was obtained -4.92 kcal/mol at the best binding site. Oleuropein has five binding sites on glycine and three binding sites on agglutinin. The binding free energy of the best site was -4.14 and -5.56 kcal, for best binding sites on glycine and agglutinin respectively. By binding these plant proteins to oleuropein, a complex can be produced, and this complex can be used for food enrichment.

***Keywords:*** Bioactive compounds, Molecular docking, Plant proteins, Encapsulation, Oleuropein

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**Harnessing the power of amino-graphene and chitosan: Novel nanohybrid supports for enzyme applications**

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**Abstract**

Composite materials and hybrid organic-inorganic systems have surfaced as advantageous platforms for the immobilization of industrial enzymes. The hybrid supports utilize the beneficial characteristics inherent in both inorganic nanoparticles and biopolymeric materials. Nanomaterials are particularly well-suited for use as enzyme supports owing to their extensive surface area. Graphene, characterized by its two-dimensional arrangement of sp² hybridized carbon atoms, exhibits distinctive properties, such as exceptional mechanical, electrical, and chemical attributes, while also being cost-effective. Nevertheless, numerous intriguing properties may be augmented via functionalization. The incorporation of bioactive compounds, including amines, onto materials offers numerous benefits. These advantages encompass enhanced stability of the active compound, improved dispersibility, increased surface area, protection from specific environmental factors, and the potential for controlled release, among others. Chitosan, the most abundant natural biopolymer, is derived from chitin, a major component of the exoskeletons of crustaceans, such as crab and shrimp shells. Chitosan is associated with excellent biological, physicochemical, antimicrobial, and nontoxic properties, making it a superior eco-friendly material. In this study, we synthesized novel nanohybrid supports by combining amino-functionalized graphene nanoplatelets (AG) and chitosan nanoparticles (CS). AG was dispersed in water and mixed with a CS solution, and then the mixture was dripped into NaOH to form AG/ AG beads. These beads were cross-linked with glutaraldehyde and washed to obtain stable AG/CS nanohybrids. Characterization with FTIR, XRD, DLS, and FE-SEM showed nanohybrid production. The synthesized AG/CS nanohybrids exhibit considerable promise as adaptable platforms for enzyme immobilization, integrating the advantageous characteristics of both inorganic and organic nanomaterials. This study demonstrates the potential for developing enzyme-based biotechnologies through the use of logically constructed inorganic-bio hybrid systems. On these nanohybrid supports, more research is necessary to fully understand enzyme loading, activity, and operational stability.

***Keywords:*** Amino-graphene, Chitosan, Nanohybrids, Enzyme Immobilization

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**Inhibitory Effects of Synthesized Porphyrins on the Aggregation of Lysozyme Protein**

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**Abstract**

Amyloid aggregation is recognized as a key pathological feature in many neurodegenerative diseases, including Alzheimer's disease, Parkinson's disease, and Huntington's disease. Amyloid beta (Aβ) and tau proteins are the most important proteins associated with Alzheimer's disease, where the aggregation of amyloid beta peptides leads to neuronal toxicity and serious damage to the functionality of nerve cells in the brain due to the consequent metal ion imbalances and oxidative stresses, to name a few, which disrupt neuronal function. Targeting the aggregation of proteins and peptides presents a promising avenue for therapeutic intervention in neurodegenerative diseases. Small molecules and compounds, such as tetrapyrroles, have been identified as potential inhibitors of amyloid formation. The aggregation of lysozyme in the presence and absence of 5-(4-carboxyphenyl)-10,15,20-triphenylporphyrin (MCTPP) and 5,10,15,20-tetrakis(4-carboxyphenyl)porphyrin (TCPP) was initially investigated using thioflavin T fluorescence assays. The results indicated that various concentrations of these compounds could inhibit lysozyme fibrillation by approximately 89% through an increase in the lag phase and a decrease in emission intensity. These findings demonstrate that MCTPP and TCPP effectively influence lysozyme fibrillation, showing a dose-dependent effect of the porphyrin compounds. To confirm the results obtained from thioflavin T fluorescence, Congo red assays, and atomic force microscopy imaging were also conducted, which verified the presence of fibrils in both the presence and absence of porphyrin compounds. UV-vis spectroscopy confirmed the structure of the porphyrin compounds and lysozyme protein, as well as potential interactions between MCTPP, TCPP, and lysozyme protein.

***Keywords:*** Degenerative diseases of the nervous system, Lysozyme, Porphyrins, Porphyrin derivatives, Amyloid aggregation

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**Investigation of the effect of melatonin on the aggregation of proteins**

Seyedeh Sara Ghorashi,Saeed Emadi\*

**Abstract**

Alzheimer's disease is one of the most common degenerative diseases of the nervous system that disrupts the cognitive and behavioral abilities of its sufferers. Alzheimer's has pathological symptoms including extracellular senile plaques mainly consist of aggregated amyloid beta fibrils, intracellular neurofibrillary tangles consisting of hyperphosphorylated tau protein, oxidative stress, and neuroinflammation. In most people with Alzheimer's, circadian rhythm disorders that are the basis of sleep-wake cycle disorders have also been seen, and there is a two-way relationship between Alzheimer's and sleep disorders. Melatonin is a hormone that regulates the sleep-wake cycle, circadian rhythm, and sleep homeostasis, it also acts as a scavenger of free radicals and an antioxidant and causes the differentiation and proliferation of nerve cells. The level of melatonin gradually decreases with age, and elderly people secrete the least amount of melatonin, which is considered as an important factor in the development of Alzheimer's. Since melatonin has anti-aggregation properties, in this study, using fluorescence and absorption spectrometry methods, fluorescence imaging, and atomic force microscopy, investigating possible interactions with the molecular docking method, and its comparative effect on the aggregation of proteins was investigated. Also, the antioxidant effects of melatonin on the treated SH-SY5Y cell line with protein aggregated were studied using cell viability, reactive oxygen species, and mitochondrial membrane potential. The results showed that melatonin, with its anti-amyloid properties, can reduce the formation of protein aggregates, and considering the docking findings, it seems that there is a molecular interaction between melatonin and the proteins. Also, the results of this research showed that due to its antioxidant properties, melatonin was able to increase survival, reduce reactive oxygen species, and reduce mitochondrial membrane damage in cells treated with aggregates.

***Keywords:*** Alzheimer's disease, Protein aggregation, Melatonin, sleep

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**Investigation of the interaction of a new platinum complex with DNA**

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**Abstract**

Platinum-based compounds such as cisplatin which can stop the growth of cancer cells and are approved by the FDA, have limited use due to the side effects. In order to develop this class of platinum drugs, cyclometalated compounds have been designed and synthesized. They are stable under physiological conditions and reach the target cells. The incorporation of phosphine ligands increases the lipophilicity of cycloplatinum complexes and their high cytotoxicity. Replacing fluorine with phosphine ligands in the synthesis of the new complex is an excellent choice to modify the electronic and hydrophobic properties. In this study, the interaction of a new platinum complex, [Pt(dfppy)Cl (Pph2 Me)] (complex 1) with calf thymus DNA was investigated using fluorescence spectroscopy. To reveal the mode of interaction between complex 1 and DNA, the competitive experiments have been carried out using several markers including ethidium bromide, thiazole orange, DAPI, methylene blue and Hoechst 33258. The main mode of the interaction of this complex with DNA was intercalation according to the competitive experiments. The fluorescence quenching data at different temperatures have been analyzed to estimate the values of the binding parameters including binding constant, Stern-Volmer constant, thermodynamic functions, and the number of binding sites for the interaction of the complex 1 with DNA. According to the values of thermodynamic functions, it was inferred that the effective forces in the interaction of this new cylcloplatinated compound with DNA are van der Waals type or hydrogen bond formation.

***Keywords:*** Platinum complexes, Cycloplatinated compounds, DNA binding, Ligand-binding

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**Beyond apoptosis: The diverse roles of Caspase-9 in cancer cell fate determination**

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**Abstract**

Apoptosis is a regulated process involving various signaling pathways and mechanisms, prominently featuring caspases, a family of proteases essential for cell death. Recent research has revealed that caspase-9, an initiator caspase in the intrinsic apoptotic pathway, also plays non-apoptotic roles in processes like differentiation and migration. This study explored the non-apoptotic functions of caspase-9 and its potential contributions in cancer cells, specifically in glioblastoma, neuroblastoma, leukemia, and breast cancer cell lines and their organoid models.

Findings showed diverse effects of caspase-9 activation across different cancers. In luminal breast cancer, it prompted apoptosis, while in tamoxifen-resistant cells, it did not cause cell death. In triple-negative breast cancer, it had anti-metastatic effects, and in glioblastoma, it induced cellular senescence; meanwhile, it fostered differentiation in leukemia and neuroblastoma cells. All organoid models exhibited decreased features associated with aggressive epithelial-mesenchymal transition (EMT). Moreover, a data mining survey suggested a link between downregulation of caspase-9 and aggressive traits in breast cancer. These insights indicate that caspase-9 activation could significantly affect cell fate in various cancers. Thus, targeted activation of caspase-9 may serve as a promising therapeutic strategy, especially for aggressive cancers characterized by EMT. Further investigation is needed to understand the underlying mechanisms and therapeutic potential of caspase-9 in cancer.

***Keywords:*** Caspase-9, Cell fate, Apoptosis, Senescence, Differentiation, Cancer cells, Organoid models

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**p53: A molecular switch determining cell fate between apoptosis and differentiation**

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**Abstract**  
Apoptosis and differentiation are critical cellular processes that share common molecular features, including, cytochrome c release and caspase activation. Despite these shared characteristics, the factors determining whether a cell undergoes apoptosis or differentiation remain poorly understood. Herein, we sought to identify the key genes regulating cell fate decisions between these two processes. We first curated gene sets related to apoptosis and differentiation from the GSEA database, narrowing our focus to genes with high frequencies. This led to the creation of refined gene sets that were analyzed using Enrichr. To validate these gene sets, we utilized 80 microarray samples from the GEO database and performed enrichment analysis. Remarkably, over 70% correlation was observed between our refined gene sets and hallmark gene sets. Further analysis revealed 16 common genes between the apoptosis and differentiation networks, with p53 exhibiting the highest betweenness centrality. The protein-protein interaction (PPI) networks were constructed using Cytoscape and merged. Network analysis identified p53 as the most critical node in the final PPI network. To explore the functional role of p53, we analyzed its activity during differentiation using ISMARA and GEO datasets. We observed transient p53 activity during the differentiation of mesenchymal stem cells, consistent with reports that p53 dynamic regulates cell fate. Our findings highlight the pivotal role of p53 in balancing apoptosis and differentiation, providing insights into its function as a critical determinant of cell fate.

***Keywords:*** Apoptosis**,** Differentiation**,** Cell fate**,** Cell signaling, p53

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**TP53: A key regulator in the decision between cellular senescence and apoptosis**

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**Abstract**

Senescence and apoptosis are distinct cellular fates with interconnected regulatory mechanisms. While apoptosis results in rapid cell death, senescence is characterized by stable cell cycle arrest and a distinct secretory phenotype. Studies suggest that cells exposed to apoptotic stimuli can undergo senescence under certain conditions. This study aimed to identify critical regulators determining cell fate choice between senescence and apoptosis. We collected the curated gene sets from the GSEA and utilized STRING database to construct and analyze the protein-protein interaction (PPI) networks for apoptosis and senescence in cells. Functional enrichment analysis using Enrichr validated the identified networks, and then PPI network analysis using Cytoscape revealed TP53 as a protein with the highest degree of interactions and a pivotal regulator influencing cell fate. Our findings consistent with other scientific reports suggest that TP53 modulates cell cycle control mechanisms, thereby impacting the decision between senescence and apoptosis. However, further investigation is warranted to elucidate the precise role of TP53 and other regulators in this cellular fate choice.

***Keywords:*** Apoptosis - Senescence - TP53 - Cell cycle

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**Enhancing Publication Retrieval in Basic Sciences: Insights from a Systematic Review on Sweet Molecules**

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**Abstract**

To investigate the structure-sweetness relationship of sweet molecules, four databases Web of Science, SCOPUS, PubMed, and FlavorDB were systematically searched for studies on sweet proteins and small sweet molecules in the SweetenersDB database. No comprehensive study was retrieved. Subsequently, a broader search using general keywords like sweetener, sweet molecules, and sweetening agents yielded 8,231 studies. Of these, only 122 studies on small molecules and 38 on sweet proteins met the criteria for investigating structure-function relationships.

Analysis revealed that studies on small sweet molecules often used diverse terminologies not found in SweetenersDB. For instance, instead of saccharin, acesulfame, or cyclamate, terms such as sulfamate, sulfonyl, or chemical formulas like RNHSO3-M+ were used, leading to few and scattered results in the initial search. Adding these terms later retrieved many related studies, making further searches unnecessary.

However, many eligible studies were either missed or excluded during initial screening because their titles, abstracts, or keywords lacked informative terms like “sweetener” or sufficient details on the structure-function relationship. Consequently, these studies were overlooked in the early stages of the search.

In conclusion, diverse expertise in basic sciences creates variability in terminology and perspectives on a topic. To ensure visibility and retrieval, it is crucial to include clear and accurate keywords and study purposes in the title, abstract, and keywords—often the only sections that catch readers' attention.

***Keywords:*** Systematic review, Basic sciences, Title, Abstract, Keyword, Skills

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**Structural changes in insulin via binding of anticancer drug of Pomalidomide**

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**Abstract**

Insulin is a peptide hormone produced by the beta cells of the pancreas that plays a critical role in regulating blood glucose levels. By binding to its specific receptors on cell surfaces, insulin can facilitate the uptake of glucose from the bloodstream into cells. It is commonly used in the treatment of type 1 and type 2 diabetes, particularly in patients experiencing elevated blood sugar levels due to deficiencies in insulin production or function. Pomalidomide is an anti-cancer drug primarily used in the treatment of multiple myeloma, a type of blood cancer. This drug suppresses the growth of cancer cells by inhibiting certain immune processes and activating caspases. In this study, the interaction of pomalidomide with insulin protein was examined to assess potential changes in the structure and function of this hormone. Fluorescence spectroscopy and ultraviolet-visible (UV-Vis) spectroscopy were employed for this purpose. Intrinsic fluorescence results indicated that the addition of pomalidomide to insulin solution can led to a significant decreasing and quenching in the fluorescence intensity of insulin, which could be attributed to structural or conformational changes in the protein. Fluorescence emission data analysis using the Stern-Volmer and the logarithmic Hill equations revealed that approximately one binding site exists for pomalidomide on insulin at different temperatures of 27 and 37 °C. This binding occurs through a static mechanism, which may indicate a specific type of interaction between the drug and the protein.

***Keywords:*** Insulin, Pomalidomide, Fluorescence Spectroscopy, UV-Visible Spectroscopy

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**Investigation of interaction and structural changes of insulin in the presence of Lenalidomide**

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**Abstract**

Insulin, a globular peptide hormone (MW 5808 Da), comprises two polypeptide chains: the A-chain (21 amino acids) and the B-chain (30 amino acids), linked by disulfide bonds. Lenalidomide as a potent immunomodulatory drug, is a less toxic analog of thalidomide and was developed to reduce side effects like peripheral neuropathy. Our main aim in the present study is to investigate the interaction and structural alterations in Insulin due to presence of different concentrations of Lenalidomide. For this purpose, we execute two different spectroscopy methods, Fluorescence and UV-Visible, to examine the interactions, structural changes and related parameters. The intrinsic fluorescence data show systematic quenching of insulin's natural emission spectrum in the presence of various concentrations of lenalidomide at both of the temperatures of 25 and 37 °C. The number of binding sites and binding constants were analyzed by using quenching data. Hill equation analysis identifies that there is one binding site on insulin for binding of lenalidomide at both of the temperatures. Also, according to Stern-Volmer equation and plots which confirm the static quenching mechanism. These results suggest lenalidomide can interact and bind with insulin protein through static quenching, offering insights into their molecular interactions and potential effects.

***Keywords:*** Insulin, Lenalidomide, Hill equation, Stern-Volmer equation

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**Application of genetic engineering in commercial enzyme Production: expression of recombinant serine protease from Virgibacillus natechei**

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**Abstract**

Hydrolysis of fish waste protein is an effective and economical strategy for obtaining valuable products with diverse applications. Fish waste, often considered a byproduct, is rich in proteins and bioactive compounds that can be transformed into high-value products such as peptides and amino acids. In recent years, researchers have prioritized green and sustainable technologies for the hydrolysis of fish-derived proteins. These approaches aim to replace traditional chemical methods, which may pose environmental and health risks, with safer and more environmentally friendly alternatives. Among these, proteolytic enzymes have emerged as a promising solution, offering high specificity, efficiency, and mild operational conditions. However, natural enzymes face significant challenges, including high production costs, limiting their large-scale industrial application. To address this limitation, modern biotechnology tools, particularly genetic engineering, are being employed to produce recombinant enzymes with enhanced properties. In the present study, the synthetic gene encoding serine protease, an enzyme with considerable potential for protein hydrolysis, was inserted into the PET28a expression vector. This recombinant construct was then successfully introduced into the E. coli BL21(DE3) strain. The accuracy of the gene transfer was confirmed using Colony PCR, while the expression of the recombinant enzyme was evaluated through Real-Time PCR analysis. The successful production of serine protease from Virgibacillus natechei highlights its potential as a cost-effective alternative for various applications. If the purified enzyme demonstrates suitable biochemical properties, including high activity and stability, further studies may establish its viability for commercial use in industries like fisheries, waste management, and protein recovery.

***Keywords:*** Gene synthesis, Recombinant protease, *E. coli* BL21(DE3), Real-Time polymerase chain reaction

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**Design and fabrication of nanocomposite hydrogel based on polyacrylic acid containing cellulose nanocrystal and zinc sulfide nanoparticles for wound dressing application**

Ali Rokn-Rabeia,\*, Seyed Emad Hooshmandb, Bahareh Dabirmaneshb, Khosro Khajehb,\*

**Abstract**

Hydrogels are biomimetic materials that mimic the extracellular matrix of biological soft tissues. Due to that fact, using hydrogels in biomedical applications has become a rapidly expanding research area in the biomedical field. Fabrication of a wound dressing that simultaneously has proper biological and mechanical properties is a challenging issue. This work aims to exploit nanomaterials to endow appropriate mechanical and biological properties to polyacrylic-based hydrogel for wound dressing application. For this purpose, the Hydrogel was synthesized with polyacrylic acid (PAA) as the base polymer, including cellulose and zinc sulfide nanoparticles. Cellulose nanoparticles were considered to improve the mechanical properties and zinc sulfide nanoparticles to give antibacterial properties to the wound dressing. Analysis such as SEM, FTIR, and Thermogravimetric analysis (TGA) were conducted to characterize the hydrogel. MTT assay confirmed that the wound dressing is biocompatible. In addition, microbiological analysis showed that the wound dressing has significant antimicrobial activity against Staphylococcus aureus and Escherichia coli. Our work introduces a biocompatible, antimicrobial nanocomposite hydrogel that may have promising clinical applications as a wound dressing material.

***Keywords:*** Hydrogel, Wound dressing, Poly acrylic acid, Zinc sulfide nanoparticle, Cellulose nanocrystal

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