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1. **Chhetri A.; Roy M.;** Mishra P.;Halder A.K.; Basak S.; Gangopadhyay A.; Saha A.; Bhattacharya P., Genetic algorithm-de novo, molecular dynamics and MMGBSA based modelling of a novel Benz-pyrazole based anticancer ligand to functionally revert mutant P53 into wild type P53, Molecular Simulation, 2023, 49, 678, 10.1080/08927022.2023.2185079. I.F. 1.9
2. **Nandi A.;** Das A.; Dey Y.N.; Roy K.K., The Abundant Phytocannabinoids in Rheumatoid Arthritis: Therapeutic Targets and Molecular Processes Identified Using Integrated Bioinformatics and Network Pharmacology, Life, 2023, 13, NA, 10.3390/life13030700. I.F. 3.2
3. **Paul M.;** Pramanik S.D.; Sahoo R.N.; Dey Y.N.; Nayak A.K., Dental delivery systems of antimicrobial drugs using chitosan, alginate, dextran, cellulose and other polysaccharides: A review, International Journal of Biological Macromolecules, 2023, 247, NA, 10.1016/j.ijbiomac.2023.125808. I.F. 7.7
4. **Chattaraj B.;** Nandi A.; Das A.; Baidya A.; Mahata S.; Chowdhury A.; Mitra S.; Roy S.; Chakraborty S.; Dey Y.N., Enhydra fluctuans Lour. aqueous extract inhibited the growth of calcium phosphate crystals: An in vitro study, Food Chemistry Advances, 2023, 2, NA, 10.1016/j.focha.2023.100287. I.F. 0
5. **Chattaraj B.;** Khanal P.; **Nandi A.;** Das A.; Sharma A.; Mitra S.; Dey Y.N., Network pharmacology and molecular modelling study of Enhydra fluctuans for the prediction of the molecular mechanisms involved in the amelioration of nephrolithiasis, Journal of Biomolecular Structure and Dynamics, 2023, 41, 15400, 10.1080/07391102.2023.2189476. I.F. 2.7
6. **Nandi A.; Nigar T.;** Das A.; Dey Y.N., Network pharmacology analysis of Plumbago zeylanica to identify the therapeutic targets and molecular mechanisms involved in ameliorating hemorrhoids, Journal of Biomolecular Structure and Dynamics, 2023, NA, NA, 10.1080/07391102.2023.2280681. I.F. 2.7
7. **Chattaraj B.; Nandi A.;** Das A.; Sharma A.; Dey Y.N.; Kumar D.; R M., Inhibitory activity of Enhydra fluctuans Lour. on calcium oxalate crystallisation through in silico and in vitro studies, Frontiers in Pharmacology, 2023, 13.0, NA, 10.3389/fphar.2022.982419. I.F. 4.4
8. Dhibar M.; Chakraborty S.; **Kundu A.; Laha P.,** Chemistry Characterization and Application of Nanocrystals-based Drug Delivery System: Present to Future Perspective, Pharmaceutical Nanotechnology, 2023, 11, 265, 10.2174/2211738511666230109151410. I.F. 0
9. Chakraborty S.; Dhibar M.; **Das A.;** Swain K.; Pattnaik S., A Critical Appraisal of Lipid Nanoparticles Deployed in Cancer Pharmacotherapy, Recent Advances in Drug Delivery and Formulation, 2023, 17, 132, 10.2174/2667387817666230726140745. I.F. 0
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A Critical Appraisal of Lipid Nanoparticles Deployed in Cancer Pharmacotherapy

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PMID: 37493164 DOI: 10.2174/2667387817666230726140745

Abstract

Treatment modalities of various cancers and the delivery strategies of anticancer agents have evolved significantly in the recent past. The severity and fatality of the disease and hurdles to the effective delivery of therapeutic agents have drawn the attention of researchers across the world for proposing novel and effective drug delivery strategies for anticancer therapeutics. Attempts have been made to propose solutions to the diverse limitations like poor pharmacokinetics and higher systemic toxicities of the traditional delivery of anticancer agents. Nanotechnology-based drug delivery systems including lipid-based nanocarriers have demonstrated significant efficiency in this scenario. The review critically assessed the different types of lipid nanocarrier systems for the effective and optimal delivery of anticancer therapeutic agents. The diverse synthesis approaches are discussed for the laboratory scale and commercial development of different categories of lipid nanocarriers. Further, their application in anticancer drug delivery is illustrated in detail followed by a critical appraisal of their safety and toxicity.

Keywords: Lipid-based nanocarriers; cancers; liposomes; nanomedicine; nanotoxicity; solid lipid nanoparticles..

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Chemistry Characterization and Application of Nanocrystals-based Drug Delivery System: Present to Future Perspective

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Abstract

With the development of new technologies, various drugs with higher efficacy have been found, but their therapeutic use is still limited owing to poor water solubility, which leads to poor systemic bioavailability. Currently, about 40% of newly discovered drugs have a solubility issue. It is a major challenge for formulation scientists to overcome this problem and make a robust and effective formulation. One such unique approach is to formulate the drug as nanocrystals which alter the physical characteristics of the drug, resulting in the development of a novel formulation strategy for poorly soluble drugs. Nanocrystals are produced by various techniques such as top-down, bottom-up, or combination methods. Nanocrystals improve the clinical application of problematic drug molecules by decreasing the particle size, enhancing the dissolution rate and reducing the dose requirement, etc. This approach is not only improving the bioavailability of the drug but also facilitates the drug targeting to specific sites due to its feasibility of surface modification and all administration routes. This article deals with the various aspects of nanocrystals including chemistry, production, stabilization, characterization, and application in the field of pharmacy.

Keywords: Solubility; dissolution; drug targeting; drug targeting solubility; nanocrystals; systemic bioavailability.

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Enhydra fluctuans Lour. aqueous extract inhibited the growth of calcium phosphate crystals: An *in vitro* study

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ABSTRACT

Enhydra fluctuans Lour. is consumed by various tribes in their ethnomedicinal practices for the treatment of kidney stones and urinary problems. However, no scientific studies were conducted to evaluate its effect on crystal growth. Hence, the present study proposed to investigate the effect of aqueous extract of whole plant of standardized *E. fluctuans* (AEEF) on the growth of calcium phosphate (brushite) crystals. Attempts were also made to evaluate the effect of *in vitro* free radical scavenging and antimicrobial activities of AEEF. *In vitro* studies indicated that AEEF (50, 100, and 200 µg/mL) exhibited an inhibitory role on brushite crystal growth. The average length of the deposited brushite crystals was decreased by citric acid ($1 molL^{-1}$) and AEEF (200, 100, and 50 µg/mL) till day 8. Results showed that AEEF (200 and 100 µg/mL) and citric acid significantly ($P<0.001$) decreased the crystal bed as compared to the control on day 8 of the study. AEEF showed an antimicrobial effect against *Staphylococcus aureus* and exhibited antioxidant activity. In conclusion, the aqueous extract of the whole plant of *Enhydra fluctuans* was found effective in the inhibition of brushite crystals. Further, *in vivo* studies along with molecular studies and bioactivity-guided fractionation are required to strengthen its antilithiatic effect along with identifying the bioactive compounds and the mechanism of action involved therein.

1. Introduction

The accumulation of stones in the kidney and urinary system is known as urolithiasis which has affected about 10 to 12 percent of the world population (Ghodasara et al., 2010). The renal stones may be divided into two subtypes *i.e.* calcareous stones which include calcium oxalate and calcium phosphate and the other subtype type is non-calcareous stones which include uric acid, and struvite (infection stone by protease bacteria), cystine, and uric acid stones (Parmar, 2004). Free radicals/ROS are implicated in several infectious conditions like urolithiasis (Boonla, 2018) and urinary tract infections (Kurutas et al., 2005), etc. They are generated either due to microbial actions or the biochemical reactions in the body. These molecules further aggravate the disease conditions leading to permanent pathologies. The availability of modern medicine in urolithiasis is sparse and hence, due to the scarcity of modern medicine and the occurrence of enormous adverse effects and side effects of the current limited antilithiatic agents like thiazide or alkali-citrate, the research on traditional medicine especially in kidney stones is only the choice which is rising tremendously in the last decade. Previous studies showed the beneficial effects of many herbal drugs on urolithiasis as revealed in various experimental studies (Sharma et al., 2016; Sikarwar et al., 2017). Though traditional and folkloric medicines are highly efficacious, their uses are limited due to a lack of knowledge and scientific evidence for their probable molecular mechanism due to the presence of multi constituents.

Enhydra fluctuans Lour. (Synonym: Helencha) belongs to the family Asteraceae, is a well-known plant is specifically a tropical and subtropical plant and mainly found in India, Bangladesh, Srilanka, Burma, and other southeast Asian countries. Previous studies revealed that *E. fluctuans* possesses antioxidant, analgesic anti-inflammatory, anti-cancer, anti-diarrheal, anthelmintic, antimicrobial, CNS depressant, cytoprotective, hepatoprotective, and thrombolytic activities (Ijaz & Roy, 2014). In ethnomedicinal practices, the decoction of the whole plant of *E. fluctuans* is consumed by various tribes of the Northeast region of India and Bangladesh for the treatment of kidney stones and urinary problems (Lokendrajit et al., 2011; Ahmed et al., 2016, 2017). Recently, the network pharmacology studies predicted the mechanisms of *E. fluctuans* on amelioration of nephrolithisis (Chattaraj et al., 2023a) while the *in vitro* studies revealed that *E. fluctuans* aqueous extract exhibited an inhibitory effect on calcium oxalate crystallization (Chattaraj et al., 2023b). However, no scientific studies were carried out to delineate its influence on

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Network pharmacology and molecular modelling study of *Enhydra fluctuans* for the prediction of the molecular mechanisms involved in the amelioration of nephrolithiasis

Bornika Chattaraj, Pukar Khanal, Arijit Nandi, Anwesha Das, Amit Sharma, Soumya Mitra & Yadu Nandan Dey

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Article

The Abundant Phytocannabinoids in Rheumatoid Arthritis: Therapeutic Targets and Molecular Processes Identified Using Integrated Bioinformatics and Network Pharmacology

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Abstract: The endocannabinoid system consists of several phytocannabinoids, cannabinoid receptors, and enzymes that aid in numerous steps necessary to manifest any pharmacological activity. It is well known that the endocannabinoid system inhibits the pathogenesis of the inflammatory and autoimmune disease rheumatoid arthritis (RA). To the best of our knowledge, no research has been done that explains the network-pharmacology-based anti-rheumatic processes by focusing on the endocannabinoid system. Therefore, the purpose of this study is to further our understanding of the signaling pathways, associated proteins, and genes underlying RA based on the abundant natural endocannabinoids. The knowledge on how the phytocannabinoids in *Cannabis sativa* affect the endocannabinoid system was gathered from the literature. SwissTarget prediction and BindingDB databases were used to anticipate the targets for the phytocannabinoids. The genes related to RA were retrieved from the DisGeNET and GeneCards databases. Protein–protein interactions (high confidence > 0.7) were carried out with the aid of the string web server and displayed using Cytoscape. The Kyoto Encyclopedia of Genes and Genomes (KEGG) metabolic pathway analysis was used to perform enrichment analyses on the endocannabinoid–RA common targets. ShinyGO 0.76 was used to predict the biological processes listed in the Gene Ontology (GO) classification system. The binding affinity between the ligand and the receptors was precisely understood using molecular docking, induced-fit docking, and a molecular dynamics simulation. The network pharmacology analyses predicted that processes like response to oxygen-containing compounds and peptodyl-amino acid modification are related to the potential mechanisms of treatment for RA. These biological actions are coordinated by cancer, neuroactive ligand–receptor interaction, lipids and atherosclerosis, the calcium signaling pathway, and the Rap1 signaling pathway. According to the results of molecular docking, in the context of RA, phytocannabinoids may bind to important target proteins such PIK3CA, AKT1, MAPK9, PRKCD, BRAF, IGF1R, and NOS3. This entire study predicted the phytocannabinoids' systemic biological characteristics. Future experimental research is needed, however, to confirm the results so far.

Keywords: cannabis; *Cannabis sativa*; endocannabinoid system; inflammation; network pharmacology

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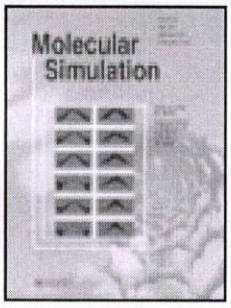
1. Introduction

Although inflammation is a typical reaction to tissue damage, it can become out of control and cause further problems. Specific soluble pro-inflammatory mediators, including cytokines or chemokines, prostaglandins, and leukotrienes, are produced as a result of an inflammatory reaction [1]. Many acute and chronic disorders are made worse by persistent inflammation. Rheumatoid arthritis (RA) is just one of the many chronic inflammatory



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Genetic algorithm-*de novo*, molecular dynamics and MMGBSA based modelling of a novel Benz-pyrazole based anticancer ligand to functionally revert mutant P53 into wild type P53

Ashik Chhetri, Moloy Roy, Puja Mishra, Amit Kumar Halder, Souvik Basak, Aditi Gangopadhyay, Achintya Saha & Plaban Bhattacharya

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Review

Exploring the Complex Relationship between Diabetes and Cardiovascular Complications: Understanding Diabetic Cardiomyopathy and Promising Therapies

Nilanjan Ghosh [1,†], Leena Chacko [2,†], Hiranmoy Bhattacharya [3], Jayalakshmi Vallamkondu [4], Sagnik Nag [5], Abhijit Dey [6], Tanushree Karmakar [7], P. Hemachandra Reddy [8], Ramesh Kandimalla [9,*] and Saikat Dewanjee [3,*]

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Abstract: Diabetes mellitus (DM) and cardiovascular complications are two unmet medical emergencies that can occur together. The rising incidence of heart failure in diabetic populations, in addition to apparent coronary heart disease, ischemia, and hypertension-related complications, has created a more challenging situation. Diabetes, as a predominant cardio-renal metabolic syndrome, is related to severe vascular risk factors, and it underlies various complex pathophysiological pathways at the metabolic and molecular level that progress and converge toward the development of diabetic cardiomyopathy (DCM). DCM involves several downstream cascades that cause structural and functional alterations of the diabetic heart, such as diastolic dysfunction progressing into systolic dysfunction, cardiomyocyte hypertrophy, myocardial fibrosis, and subsequent heart failure over time. The effects of glucagon-like peptide-1 (GLP-1) analogues and sodium-glucose cotransporter-2 (SGLT-2) inhibitors on cardiovascular (CV) outcomes in diabetes have shown promising results, including improved contractile bioenergetics and significant cardiovascular benefits. The purpose of this article is to highlight the various pathophysiological, metabolic, and molecular pathways that contribute to the development of DCM and its significant effects on cardiac morphology and functioning. Additionally, this article will discuss the potential therapies that may be available in the future.

Keywords: diabetes mellitus; diabetic cardiomyopathy; heart failure; hyperglycemia; insulin resistance; lipotoxicity

1. Introduction

Diabetes mellitus (DM) and its associated pathophysiological events have emerged as a leading risk factor for the development of diabetes cardiomyopathies (DCM) and subsequent heart failures, posing serious health concerns worldwide. The identification of a causal link between cardiomyopathy and diabetes within the cardio-renal metabolic

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Inhibitory activity of *Enhydra fluctuans* Lour. on calcium oxalate crystallisation through *in silico* and *in vitro* studies

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The decoction of the whole plant of *Enhydra fluctuans* is used ethno medicinally by various tribes for the treatment of kidney stones and urinary problems. However, no scientific studies were carried out to delineate its influence on urinary stone formation and crystallisation. Hence, the present study is proposed to investigate the effect of the aqueous extract of *Enhydra fluctuans* extract on *in vitro* crystallisation of calcium oxalate. The present study also evaluated. *in silico* studies of the metabolites with the target proteins present in the renal calcium oxalate stone matrix. The plant material was subjected to decoction to obtain an aqueous extract. The effect of the extract on calcium oxalate crystallization was evaluated by *in vitro* nucleation and aggregation assays. Further, the metabolites present in *E. fluctuans* were mined from the existing literature and their number was found to be 35. The selected 35 metabolites of *E. fluctuans* were subjected to molecular docking with the 5 proteins which are known to be responsible for calcium oxalate crystal growth. Results of *in vitro* studies indicated that the extract (50, 100, and 200 µg/mL) and standard drug cystone (1,000 µg/mL) exhibited an inhibitory role in the nucleation process where the percentage inhibitions were 52.69, 43.47, 21.98, and 31.67 µg/mL respectively. The results of molecular docking studies revealed that 2 out of 35 metabolites i.e. Baicalein-7-O-diglucoside and 4′,5,6,7-Tetrahydroxy-8-methoxy isoflavone-7-O-beta-D- galactopyranosyl-(1→3)-O-beta-D-xylopyranosyl-(1→4)- O-alpha-L-rhamnopyranoside showed modulatory effects on the four renal stone matrix-associated protein (Human CTP: Phosphoethanolamine Cytidylyltransferase (Protein Data Bank ID: 3ELB), UDP glucose: glycoprotein glucosyltransferase 2 (Gene: UGGT2) (AlphaFold) and RIMS-binding protein 3A (Gene: RIMBP3) (AlphaFold), and Ras GTPase activating-like protein (PDB: 3FAY) based on their docking scores which indicates that they may inhibit the crystallization process. Findings from this study show that *Enhydra fluctuans* may be effective in the prevention of the crystallization of calcium oxalate. However, further, *in vivo* studies as well as molecular studies are needed to be conducted to confirm and strengthen its anti-urolithiatic activity and to elucidate the possible mechanism of action involved therein.

KEYWORDS

calcium oxalate, crystallization, *Enhydra fluctuans*, Asteraceae, molecular docking, kidney stones

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Dental delivery systems of antimicrobial drugs using chitosan, alginate, dextran, cellulose and other polysaccharides: A review

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ABSTRACT

Dental caries, periodontal disease, and endodontic disease are major public health concerns worldwide due to their impact on individuals' quality of life. The present problem of dental disorders is the removal of the infection caused by numerous microbes, particularly, bacteria (both aerobes and anaerobes). The most effective method for treating and managing dental diseases appears to be the use of antibiotics or other antimicrobials, which are incorporated in some drug delivery systems. However, due to their insufficient bioavailability, poor availability for gastrointestinal absorption, and pharmacokinetics after administration *via* the oral route, many pharmaceutical medicines or natural bioactive substances have limited efficacy. During past few decades, a range of polysaccharide-based systems have been widely investigated for dental dug delivery. The polysaccharide-based carrier materials made of chitosan, alginate, dextran, cellulose and other polysaccharides have recently been spotlighted on the recent advancements in preventing, treating and managing dental diseases. The objective of the current review article is to present a brief comprehensive overview of the recent advancements in polysaccharide-based dental drug delivery systems for the delivery of different antimicrobial drugs.

1. Introduction

The commonly occurring dental conditions in human are periodontal disorders including gingivitis and periodontitis, which are caused by caries [1]. Dental caries is a widespread issue that affects people of all ages, and natural polysaccharides may be able to help in repairing cavities caused by microbial colonization and demineralization [2]. Periodontitis is a typical diseased dental condition by bacterial pathogens and immune system reactions, which results in toxin releasing [1]. Immune cells become engaged during the chronic stage, producing the various cytokines and reactive oxygen species (ROSs), which cause the breakdown of bone and periodontal fibers. Similarly, the application of nanotechnology may be able to overcome the difficulties associated with the treatment of oral candidiasis, a *Candida albicans* infection, which currently relies on expensive, unpleasant, and potentially hazardous medications [3]. For the localized treatment of dental disorders affecting the oral cavity including mouth, numerous pharmaceutical dosage forms have been designed and investigated [4]. The shorter retention duration in the oral cavity caused by several issues (like salivation, intermittent swallowing, consumption of foods, abrasion by the movement of soft tissue, *etc.*), is a drawback of these conventional systems. The available conventional therapy includes the procedures of mechanical plaque control, which take more time, demand highly skilled technicians, and cause patients to experience varied degrees of discomfort [5]. However, the systemic antibiotic-therapy can be crucial in the control of periodontal pathogens present in other areas of the mouth from where they may translocate to the periodontal site as well as in the eradication of pathogenic bacteria that infiltrate gingival tissue. Numerous systemic dosages of antibiotics have revealed a number of negative effects, such as insufficient concentrations of antibiotics at the location of the periodontal pocket [6]. Due to the drug's thousand-fold dilution, an adequate concentration of antibiotics at the action site is not attained, which results in a lower benefit-to-risk ratio, a quick drop in plasma of antibiotics concentrations to sub-therapeutic levels, the microbial resistance development, and peak plasma concentration of antibiotics [7].

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Network pharmacology analysis of *Plumbago zeylanica* to identify the therapeutic targets and molecular mechanisms involved in ameliorating hemorrhoids

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