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Current Topics in Medicinal Chemistry, **2021**, *21*, 1337-1359

REVIEW ARTICLE

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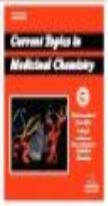
Exploring the COVID-19 Potential Targets: Big Challenges to Quest Specific Treatment



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Abstract: *Background:* The novel strain SARS-CoV-2 of coronavirus diseases (COVID-19) became pandemic at the end of 2019 with an unprecedented global crisis by infecting around 11 million people in more than 200 countries. The condition has now been provoked by the demand, supply, and liquidity shocks that COVID-19 has attacked the lives of a vast population.

Objectives: Researchers are therefore trying to encode and understand the viral genome sequence along with various potential targets to explore the transmission mechanism and the mode of treatment for COVID-19. The important structural proteins such as nucleocapsid protein (N), membrane protein (M), an envelope protein (E), and spike protein (S) related to COVID-19 are discussed in this manuscript.

Methods: The topology of these various targets has been explored utilizing structure-based design and crystallographic studies.

Results: The literature reported that the N-protein processes the viral genome to the host cell during replication. The "N-terminal domain" and "C-terminal domain" contribute towards localization in the endoplasmic region and dimerization respectively. The M protein determines the shape of coronavirus and also assists the S protein to integrate with the Golgi-endoplasmic region complex leading to the stabilization of the virion. The smallest hydrophobic viroporin termed "E" takes part in morphogenesis and pathogenesis during intracellular infection. The viral spike (S) protein attaches the cellular receptors and initiates virus-cell membrane fusions. The main protease in the proteolytic process during viral gene expression and replication has also been discussed.

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Current Drug Targets, 2021, *22*, 2006-2020

REVIEW ARTICLE

Exploring Spike Protein as Potential Target of Novel Coronavirus and to Inhibit the Viability Utilizing Natural Agents

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Abstract: ***Background:*** By the end of 2019, the sudden outbreak of the novel coronavirus disease (COVID-19) has become a global threat. It is called COVID-19 because it was caused by the novel coronavirus (SARS-COV-2) in 2019. A total of 1.9 M deaths and 87.9 M cases have been reported all over the world, where 49M cases have recovered so far. Scientists are working hard to find chemotherapeutics and vaccines for COVID-19. Mutations in SARS-CoV-2 have been observed in a combination of several hazardous stresses, making them more resistant and beneficial. So to break down the viral system, the disease targets are examined.

Objective: In today's review, a comprehensive study of spike protein explains the main purpose of the novel coronavirus and how to prevent the spread of the disease virus cross-transmission from infected to a healthy person.

Methods: Covid-19 has already been declared a pandemic by the World Health Organization (WHO) due to its result in causing death and severe illness globally. SARS-CoV-2 is highly contagious; however, the intermediate host of the novel coronavirus is not clear. To explore the mechanisms of disease, one of the viral targets, such as the spike protein that binds to human cells and causes the disease by altering its genetic structure which is considered along with potential inhibitors.

Results: It has been shown that the interaction of receptor-binding domain (RBD) protein of SARS- CoV-2 spike and the angiotensin-converting enzyme 2 (ACE2) host receptor and further replication of coronavirus spike protein causes its invasion in the host cell. The human Lymphocyte antigen 6 complex, Locus E (LY6E), inhibits the entry of CoV into host cells by interfering with the human gene, inducing spike protein-mediated membrane fusion. Some natural formulations have also been shown to prevent spike protein from binding to the host cell.

Conclusion: With the development of the LY6E gene activator that can inhibit spike protein-ACE2-mediated membrane fusion, new opportunities for SARS-CoV-2 treatment may emerge. Existing antiviral fusion inhibitors and natural compounds targeting spike resistance can serve as a template for further SARS-CoV-2 drug formulation.

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Combinatorial Chemistry & High Throughput Screening, 2021, *24*, 1628-1643

RESEARCH ARTICLE

A Quality by Design Approach of Metronidazole Bigel and Assessment of Antimicrobial Study Utilizing Box-behnken Design

Harekrishna Roy[1,*], Sudhir Maddela[1,*], Alekhya Munagala[1], Shaik Abdul Rahaman[1] and Sisir Nandi[2]

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Abstract: ***Objective*:** The present investigation aimed to prepare metronidazole (MTZ) topical bigel for the effective delivery of MTZ and to study the effect of applied variables as per statistical design. The study also signifies the implementation of the statistical method using the Quality by Design technique for MTZ bigel.

***Methods*:** The MTZ bigels were prepared as per the runs suggested by Box Behnken design (BBD) using statistical software. A total of 28 runs were suggested by the BBD, considering sodium carboxymethylcellulose (Na CMC), guar gum, hydrogel and RPM as independent variables. The prepared bigels were evaluated for organoleptic properties, percentage drug content, spreadability, viscosity, percentage *in-vitro* drug release, and antimicrobial efficacy. Model selectivity was ascertained by *p*-value considering responses along with predicted R^2 and adjusted R^2 values.The fitting of model was ascertained by F-value as well as "lack of fit" was carried out to find out the suitability of the experimental design. Furthermore, the characteristic distribution of data was ascertained by the "normal plot of residual" method. The compatibility of MTZ and excipients in bigels was confirmed by FTIR and the crystalline nature of MTZ in formulations was studied by DSC and XRD studies. Furthermore, the dispersion of bigel was assessed by the SEM study.

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Current Drug Therapy, 2022, *17*, 56-70

RESEARCH ARTICLE

Poloxamer based Urapidil Loaded Chitosan Microparticle in Approach to Improve the Mechanical Strength by Tensile Strength and Entrapment Determination

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Abstract: ***Background:*** The literature review has highlighted the issues related to the poor mechanical strength of chitosan-based microparticles. In an attempt to resolve the drawbacks, the microparticles were prepared with a suitable combination of poloxamer-188 (pluronic) and chitosan-based hydrogels.

Objective: The current study dealt with urapidil-loaded chitosan microparticles incorporating chitosan-based hydrogels and small polyanionic electrolytes. The mechanical strength was ascertained by entrapment efficiency and texture analyzer.

Methods: Chitosan-based hydrogels and the combination of poloxamer and further microparticles were prepared by the counter-ion aggregation technique in a polyanionic electrolyte medium (20 % w/v). During the preparation, poloxamer was incoporated to improve the mechanical strength, which was ascertained in terms of adhesive strength (tensile strength) by texture analyzer and entrapment efficiency. The prepared microparticles were also subjected to micrometric studies, swelling index, surface morphology study, drug-polymer interaction study, and zeta analysis.

Results: A remarkable increase in entrapment efficiency (maximum of 78.56 % from SSP4) was observed with the progressive increase in poloxamer-188. In addition to that, the adhesive strength was also studied by a texture analyzer for all microparticles. Sodium citrate-based products exhibited superior adhesive strength values than sodium sulfate- and sodium tripolyphosphate-based products, indicating the significance of incorporating poloxamer-188. A significant finding was also recorded for the swelling properties at microenvironmental pH attributed to polyanions. It was observed that sodium TPP microparticles continued to swell in a phosphate buffer of pH 6.8. Zeta value was found to be maximum with -5.2 mV; however, it could further be improved by adding electrolytes. TPP4 showed a comparatively larger particle size of 8.07 µm. Polydispersity index value revealed homogenous dispersion of microparticles. SEM study revealed prominent porous surfaces for sodium tripolyphosphate microparticles.

Conclusion: The study revealed that the addition of poloxamer-188 improved the mechanical strength, identified by entrapment efficiency and texture analysis. SCP4 microparticle was found to be the best formulation among all.

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Evaluation of Antihyperlipidemic activity of leaves of Cassia tora

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ABSTRACT:

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Original Article

A Novel Stability Indicating Method for Determination of Major Alkaloid in Black Pepper by RP-HPLC in Different Pharmaceutical Dosage Forms

Yenduri Suvarna[1,*], Shaik Abdul Rahaman[2], Arram Madhavi[3]

ABSTRACT

Background: Piperine is the major alkaloid found in the fruits of Black pepper. Recent studies revealed the antiurolithiatic effect of piperine. So, an attempt was made to develop an analytical method for the assay of Piperine in the formulated dosage forms. **Objectives:** The present study was done with the aim of developing a simple, accurate, precise and sensitive RP-HPLC method for estimation of Piperine in different dosage forms. **Materials and Methods:** Some trials were performed during method development using different solvents, mobile phase compositions and flow rate for the estimation of piperine in the dosage form. The developed optimized method was validated as per ICH guidelines and was employed to estimate the amount of piperine in the given dosage form. **Results:** The optimized chromatographic conditions were achieved using BDS C8 column with mobile phase having of water: Acetonitrile in 50: 50 ratio at 1.0ml/min flow rate. Detection was observed at 247nm using PDA detector. The retention time obtained for piperine peak was found to be 2.4 min. **Conclusion:** The analytical method which was developed for estimation of piperine is simple, rapid, economic, specific, precise, stable and can be successfully employed for its estimation

Yenduri Suvarna[1,*],
Shaik Abdul Rahaman[2],
Arram Madhavi[3]

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FORMULATION AND EVALUATION OF POLYHERBAL AIR AND HAND SANITIZER

Dr.Goday swapna *[1],P.Teja[2] ,V.Nandini[3], P.Sri Hyma[4], N.Manoj[5]

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Contact No: 8121226766

Abstract

The main aim for this preparation of poly herbal hand sanitizer formulation and evaluation is for "work place hygiene". Three different types of herbs are used in this preparation ' Azadirachta

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Pharmaceutical Sciences

Volume 11 Issue 4, July 2021 Pages:19-24

A Comprehensive Knowledge on Review of Indole Derivatives

Padmavathi Sakinala, Vemula Mounika, Komre Gangabai, Kattupalli Sathvika, Kondamudi Saikumar, Lagadapati Lakshman

[View PDF]

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Abstract:

The aim of the present review is to review synthesis and biological significance of indole derivatives. Most of the indole derivatives has varied pharmacological activities. Indole is an aromatic heterocyclic ring, which is commonly synthesized from Fischer- Indole synthesis from phenyl hydrazine and pyruvic acid. Indole undergoes electrophilic substitution reaction at position-3. It was synthesized from Batcho synthesis, Fukuyama- indole synthesis and Gassmann indole synthesis. Indole is a versatile and privileged heterocyclic ring with wide range of pharmacological activities. A plenty of research work was undertaken to synthesis and various therapeutic prospective of this moiety. The various activities of indole derivatives are Anticancer, anticonvulsant,

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A Review on a determination of Eleven pesticides in cucumber by a multi-residue GC-MS method

Sakinala padmavathi[1], K. Steli Seles [1], K.SaiDurgaBhavani, B.Labthadevi, D.Shainy grace, V.Sairamya [illegible]

Department of Pharmaceutical Analysis, Nirmala College of Pharmacy, Atmakur, Mangalagiri-522503

Abstract:

Pesticides are chemical compounds that are used to kill pests consisting of insects, rodents, fungi, and undesirable plant life (weeds). Pesticides are hazardous to human health and life; accumulated in the body, they may be carcinogenic, [illegible], and maybe the disruption of hormonal and enzymatic regulation. The gas chromatography-mass spectroscopy method is a combination of elements of gas-liquid chromatography and mass spectroscopy which is used to identify various substances within a test sample. GC-MS is used in environmental monitoring, analysis of food, beverage, fragrance, and is also used in geochemical and astrochemistry, clinical toxicology, etc. GC-MS is employed with helium as the carrier gas at a constant flow of 1ml/min. The oven temperature started at 75°C and remained at this temperature for 3 minutes increasing to 120°C at 5°C/minute ramp, holding at 300° for 11 minutes. The injection port was adjusted at 250°c and splitless injection mode was used and mass spectra. The most abundant ion showed no evidence of chromatographic reference. **Aim, objective**: after the acquisition of the total ion chromatogram for the mixed stock standard solution in scan mode, peaks were identified by their retention time and mass spectra. The most abundant ion that shows no evidence of chromatographic reference and had the highest signal-to-noise ratio was selected for quantification purposes. The usage of mass spectrometry, with its information-rich content, rational and specific confirmation, is advocated for monitoring pesticide residues in the complete world. Recent developments in GC-MS include an increase in the usage of triple quadrupole instruments, miniaturization, determination of pesticides in plant materials. Cucumber is a frequently consumed vegetable.

Keywords: Pesticide, spiked calibration curve, cucumber, GC-MS, multi-residue.

Introduction :

Pesticide:

Pesticides are chemical compounds that are used to kill pests consisting of insects, rodents, fungi, and undesirable plant life weeds. Definition of pesticide different with instance and countries. However, the essence of pesticide stays basic constant, i.e., it is a (mixed) substance that is toxic and environment [illegible]

SA Raheem (signature)

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Chronic Idiopathic Thrombocytopenic Purpura during the Pregnancy: A Case Report

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Case Report | doi:10.5530/jyp.2022.14.51

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Department of Pharmacology and Pharmacy Practice, Nirmala College of Pharmacy, Mangalagiri, Andhra Pradesh, INDIA.

Abstract:

A 37-year-old woman was admitted to the hospital after complaining of a petechiae rash all over her body for three days, generalized weakness, pallor, and gum bleeding in one episode, and a history of similar episodes in the past. The patient has Idiopathic Thrombocytopenic Purpura and has been on medication throughout her pregnancy. Peripheral examination reveals microcytic hypochromic anemia with thrombocytopenia, and bone marrow examination reveals an increase in the number of megakaryocytes. She received corticosteroid and antifibrinolytic treatment. Her symptoms are similar to those caused by steroids after being readmitted to the hospital. Idiopathic Thrombocytopenic Purpura appears to be an immune-mediated disease. Although Idiopathic Thrombocytopenic Purpura is a rare condition, it can be fatal, especially during pregnancy because of fetal intracranial hemorrhage.

Key words: Idiopathic Thrombocytopenia, Petechiae, Pregnancy, Megakaryocytes, Antifibrinolytic.

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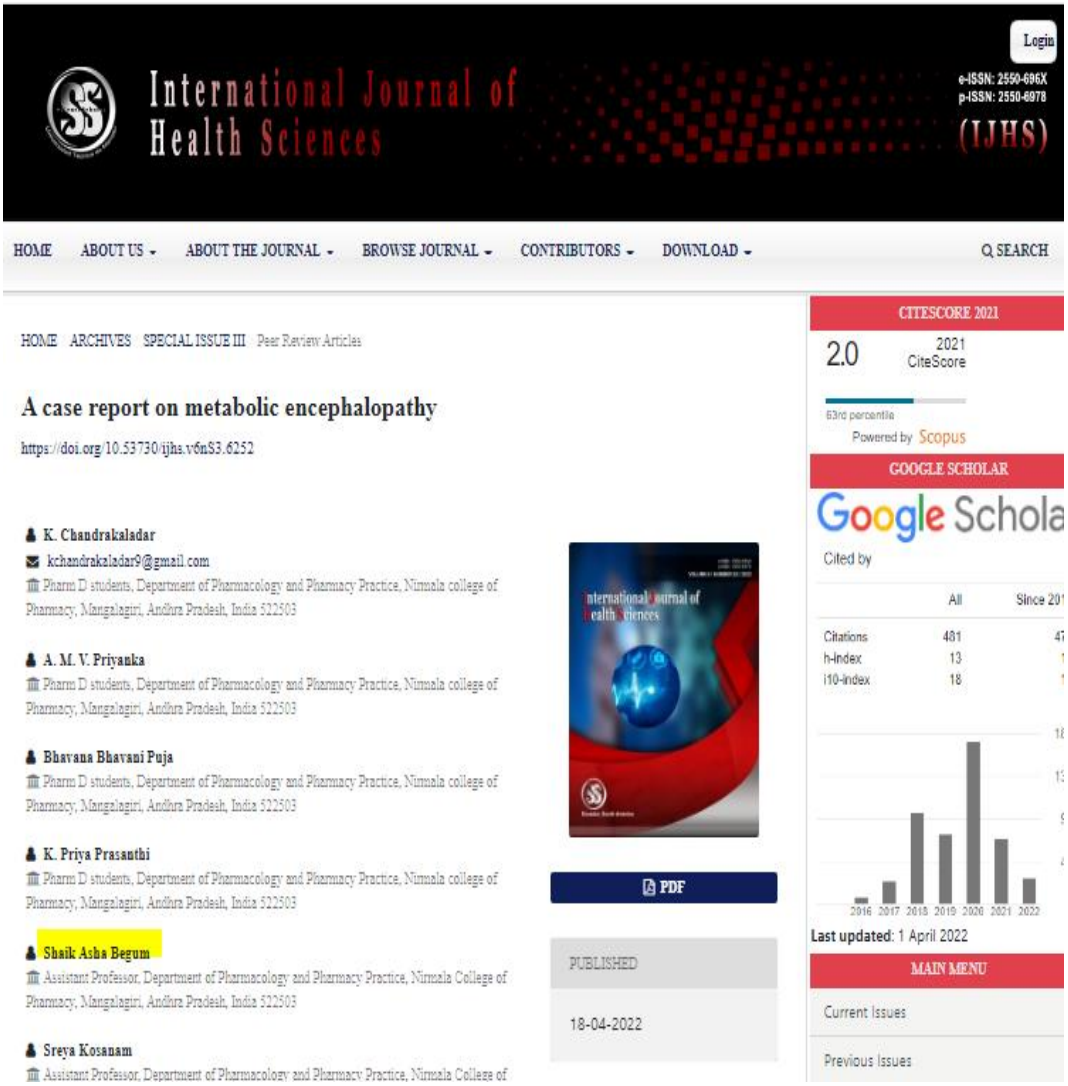

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A case report on metabolic encephalopathy

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A Case Report on Scleroderma: A Diagnostic Dilema

Ch. K. V. L. S. N. Anjana Male[1*], Hari Chandana Varikallu[2], Tirumalasetty Sai Swapna[2], N. Dileep[3], S. Hemanth Durga Prasad[4] and Sarath Nalla[5]

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Authors' contributions

This work was carried out in collaboration among all authors. All authors read and approved the final manuscript.

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Case Report

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ABSTRACT

Scleroderma is a rare heterogenous group of autoimmune fibrosing disorder that mainly exists in two forms; localized scleroderma (LS) and systemic sclerosis (SSc). It involves thickening of the skin at fingers region extending from proximal to metacarpophalangeal joints. The diagnostic criteria of scleroderma include past history of patient, symptoms of patient, serology, and skin biopsy. The morbidity and mortality are much worse for SSc with the patients are at risk for life threatening lung, heart and other visceral organ fibrosis and vasculopathy. There is no drug that can cure or stop scleroderma over fibrosis, but certain drugs regulate the symptoms associated with it and boost the patient's quality of life, particularly steroidal creams that help alleviate swelling, joint pain, loosen tight skin; blood pressure drugs that dilate blood vessels; immunosuppressive agents. If the disease is severe amputation is necessary.

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Idiopathic Thrombocytopenic Purpura in Post COVID-19 Condition: Case Study

Ch K. V. L. S. N. Anjana Male[1], Kommuri Vyduryam[2*], N. V. Yaseswi[2], V. Pravallika[2], A. Javed Akhtar[2], R. Piety Christiana[2], P. Joy Nissi[2] and K.Sravya[2]

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Authors' contributions

This work was carried out in collaboration among all authors. Author CKVLSNAM did the concept design, critical revision and editing. Authors NVY, KV and VP did the case report gathering and drafting manuscript. Literature collection, verification done by authors AJA and TND. All authors Read and approved the final manuscript.

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Case Study

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ABSTRACT

A 50 years old woman was referred to hospital with compaints of bluish black discoloration of skin or multiple ecchymosis since 6 days and skin rashes, pink changes or petechiae changes since 1 week, dark color stools since 3 days. She had a history of COVID-19 positive on past "3 months" back and she received the corticosteroids, antiviral drugs, broad spectrum antibiotics, anticoagulants, and vitamin B and C supplements. Now patient is admitted and investigated for further management. Her bone marrow examination reveals marrow cytological features are compatible with immune thrombocytopenic Purpura and peripheral examination reveals red cells are microcytic hypochromic with elongation forms, platelets are markedly reduced and elevation of CRP, reduction of the Hb, PCV, MCH, MCV, MCHC, APTT, Serum vitamin B12, Lymphocytes and

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Hyperlipidemia Condition and Novel-Drug Therapies: A Overall Study

CH. K. V. L. S. N. Anjana Male[1], V. Swathi[1], D. Sai Kumar[1*], Karishma[1] and Md. Shuaib Yunus[1]

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Authors' contributions

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Review Article

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ABSTRACT

Hyperlipidaemia is an condition that increases the chance of coronary heart disease (CHD) and atherosclerotic disease (ASHD) in blood vessels. Hyperlipidaemia occurs in response to smoking, obesity, sedentary lifestyle, and other risk factors to extend CHD. Cardiovascular disease (CVD) is the reason for death.

Hyperlipidaemia is divided into two broad classifications: Primary (familial) and Secondary (acquired).

Primary hyperlipidemia has been generated by hereditary defects and climatic factors or by undisclosed mechanisms. Secondary hyperlipidemia concern to the metabolic disorders linked with the diabetes mellitus, liver complication, thyroid, and kidney complications. Hyperlipidemia also refers to as elevated levels of lipids within the blood. Circulating lipid are carried in lipoproteins that transport the lipids to varied tissues for energy use, lipid deposition, hormone production, and steroid formation. The lipoprotein consists of esterified and unesterified cholesterol, triglycerides, phospholipids, and protein. The general public who have hyperlipidemia experience no symptoms

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Research Article
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A Review on Phytosomes- A Novel Drug Delivery System

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Abstract:
Phytopharmaceuticals are curing the world from millions and billions of years. Phytosome technology shows target ability of active plant constituents, superior efficacy and quality. This review highlights the characteristic properties of Phyto phospholipid complex along with their application in the novel natural drug delivery. Here various methods used in Phytosome preparation, advantages over conventional formulations, patents, commercial products in the market are described, which will be helpful for the researchers to carry out their future works.
Keywords: Phytoconstituents; Phospholipids; Bio-availability.

1. Introduction:

History of Phytosome:

Herbal products are used as a core medicine since ancient times to till today in most of the world's population.(Amrita I, Jadhav *et al*: 2014) .Many Pharmacological studies are going on to know the medicinal value of plant product. **Phytosome**, are complex cell-like phospholipids structures ("phyto" **means** plant, "some" **means** cell-like) and a natural active ingredient which increases absorption and bio availability of active phyto constituents both orally as well as topically.(Patel Amit *et al*:2013)The valuable components of the herbal extract are protected from destruction by digestive secretions and gut bacteria.(Sudhir Kumar *et al*:2019)Most of the biologically active constituents of plants are polar or water soluble molecules in which water soluble Phytoconstituents (like tannins, flavonoids, terpenoids etc.) are poorly absorbed due to their large size. Various herbal

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Inflammopharmacology

ORIGINAL ARTICLE

Acteoside isolated from *Colebrookea oppositifolia* attenuates I/R brain injury in Wistar rats via modulation of HIF-1α, NF-κB, and VEGF pathways

Gollapalle Lakshminarayanashastry Viswanatha[1] · Hanumanthappa Shylaja[2] · Krishnadas Nandakumar[3] · Subbanna Rajesh[4] · CH K. V. L. S. N. Anjana Male[5]

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Abstract

Aims The objective of this study was to assess the anti-stroke activity of acteoside isolated from methanolic root extract of *C. oppositifolia*

Methods Ischemia–reperfusion(I/R) brain injury was induced in Wistar rats to assess the anti-stroke activity of acteoside. Rats were pretreated with acteoside (10, 25 & 50 mg/kg, p.o.) before the induction of I/R injury. Parameters such as neurological, motor-cognitive functions were evaluated along with morphological (brain volume, infarct size), biochemical (SOD, Catalase, GSH, lipid peroxidation, TNF-α, IL-6, IL-10, ICAM-1, HIF-1α, VEGF, and NF-κB), histopathological, and gene expression studies (HIF-1α, VEGF) were performed to study the protective effect of acteoside against I/R induced brain injury.

Results I/R injury caused significant deterioration of neurological ($p < 0.01$), motor ($p < 0.01$) and cognitive ($p < 0.01$) functions, associated with increase in the brain volume ($p < 0.01$), and infarct size ($p < 0.01$); increase in the levels of MDA, TNF-α, IL-6, ICAM-1, HIF-1α, VEGF, and NF-κB along with significant decrease in SOD, catalase, GSH, and IL-10 ($p < 0.01$ for all parameters) compared to Sham control group. Histology of brain tissue of disease control group exhibited significant vascular changes, neutrophil infiltration, cerebral oedema, and necrosis of the neuronal cells. Further, the gene-expression studies showed significant increase in the HIF-1α ($p < 0.01$) and VEGF ($p < 0.01$) mRNA levels in the I/R control compared to Sham control. Interestingly, the acteoside (10, 25 & 50 mg/kg) has prevented the neurological, motor and cognitive dysfunctions, along with inhibiting the morphological, biochemical, histological and gene expression changes induced by I/R-injury ($p < 0.05$ for 10 mg; $p < 0.01$ for 25 & 50 mg/kg of acteoside for all the parameters).

Conclusion These findings suggest that acteoside possess potent anti-stroke activity through modulation of HIF-1α, NF-κB, and VEGF pathway along with its potent antioxidant activity.

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Interactive Effect of Seeds of *Coriandrum Sativum L.* With Glimepiride in Streptozotocin-Induced Diabetic Rats

Uppuluri Spandana, Adikay Sreedevi and Kaveripakam Sai Sruthi

[View PDF]

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Abstract:

Diabetes mellitus is a serious and most prevailing glycemic disorder mainly managed by using allopathic medicines. Due to various side effects of allopathic drugs, till today medicinal plants were widely used in treating diabetes. Among them, spices like *Coriander sativum* L. play a prominent role in managing diabetes. Type-2 diabetic patients use oral hypoglycemic drugs and also follow herbal remedies. There is a probability of interactions when herb interferes with the drug action in the body. The aim of the present study was to assess the interaction of aqueous extract of seeds of *Coriandrum sativum* with oral hypoglycemic drug glimepiride in streptozotocin-induced diabetic rats. In the present study, animals were grouped into seven of six each. Group-I, Group-II, Group-III, Group-IV, Group-V, Group-VI, and Group-VII included normal control, glimepiride, *Coriandrum sativum*, diabetic control, diabetic animals treated with glimepiride, diabetic animals treated with *Coriandrum sativum, and* diabetic animals treated with glimepiride and *Coriandrum sativum, respectively.* Pharmacokinetic and pharmacodynamic interactions were studied. The animals treated with both *Coriandrum sativum* and glimepiride showed significant activity in pharmacokinetic parameters by increasing the levels of the maximum serum concentration (Cmax), Time taken to reach maximum serum concentration (Tmax) and Volume of distribution (Vd). Further pharmacodynamic studies showed promising hypoglycemic effects by decreasing blood

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RESEARCH ARTICLE

Analytical Method Development and Validation of Remdesivir in Bulk and Pharmaceutical Dosage Forms Using Reverse-Phase-High Performance Liquid Chromatography

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ABSTRACT

Background: Remdesivir has received significant attention for its potential application in the treatment of COVID-19, caused by severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2). Remdesivir has already been tested for Ebola virus disease treatment and found to have activity against SARS and MERS coronaviruses. The remdesivir core contains GS-441524, which interferes with RNA-dependent RNA polymerases alone. In non-human primates, following IV administration, remdesivir is rapidly distributed into PBMCs and converted within 2 h to the active nucleoside triphosphate form, while GS-441524 is detectable in plasma for up to 24 h. Nevertheless, remdesivir pharmacokinetics and pharmacodynamics in humans are still unexplored, highlighting the need for a precise analytical method for remdesivir and GS-441524 quantification. **Objectives:** The validation of a reliable UHPLC-MS/MS method for remdesivir and

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Wang resin catalyzed sonochemical synthesis of dihydropyrano[2,3-c]pyrazole derivatives and their interactions with SIRT1

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SIRT1
In silico study

ABSTRACT

The pyrano[2,3-c]pyrazole framework was explored for the design and synthesis of compounds as potential inhibitors of SIRT1. The feasibility of this strategy was reasoned by the unique structural features of this scaffold and the reported cytotoxicity of compounds containing this framework. The sonochemical synthesis of target compounds was accomplished by using the Wang resin (Wang-OSO_3H) as a recoverable catalyst under eco-friendly conditions. Thus, the desired 4-substituted 6-amino-3-methyl-1,4-dihydropyrano[2,3-c]pyrazole 5-carbonitrile derivatives were prepared via a 4-component reaction of β-ketoester, hydrazine, aldehyde and malononitrile in pure water in good yields. The recyclability of the catalyst was demonstrated successfully. All the synthesized compounds were initially assessed *in silico* against the targeted protein i.e. hSIRT1 that indicated compound **5i** and **5l** along with several other compounds as possible inhibitors. Both of these compounds participated in two vital H-bond interactions with the residue GLN345 and ASN346 *in silico* that was reflected in their estimated total energy. *In vitro* assessment of these pyrano[2,3-c]pyrazoles against SIRT1 revealed encouraging inhibitory activities (> 50% inhibition) that was in agreement with the results of docking studies. Indeed, **5i** and **5l** were identified as the most active compounds in this series. The Structure-Activity-Relationship (SAR) study suggested important role of the C-4 aryl substituent along with the N-1 phenyl ring of the pyrano[2,3-c]pyrazole moiety in the SIRT1 inhibitory activities of this class of compounds. Thus, a OH or Cl group at the p-position of the C-4 benzene ring together with the N-1 phenyl moiety appeared to be beneficial for activity. Overall, the initial design and then sonochemical synthesis followed by *in silico* as well as *in vitro* studies allowed identification of pyrano[2,3-c]pyrazole based small molecules as potential inhibitors of SIRT1.

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Data Article

Molecular modeling and *In vitro* antimicrobial evaluation of some 2-Aryl-Benzoxazoles/Benzothiazole analogues containing alkyl, alkenyl and alkynyl linkages

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ARTICLE INFO

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Benzoxazole and benzothiazole derivatives
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ABSTRACT

A series of Suzuki, Heck and Sonogashira coupled Benzoxazole and Benzothiazole analogues were synthesized and screened for their in vitro antimicrobial activities, aided by molecular modeling and structure activity relationship (SAR) studies. Among the tested 31 molecules, compounds 13 (series 1), 17 (series 2) and 30 (series 3) displayed magnificent MICs (1-2μg/mL) against the antibacterial species used compared to the standard drugs. Similarly, compound 13, 17, 22, 26 and 30 also displayed similar inhibition properties (1-2μg/mL) against fungal strains used. Further, these results were supported by molecular docking studies demonstrating excellent binding affinities of -85.84 Kcal/mol and -113.57 Kcal/mol respectively for compound 13 (series 1) with 3LD6 and 6E2T proteins. Similarly, few other compounds also exhibited excellent docking scores e.g. -99.32 Kcal/mol, -85.26 Kcal/mol for series 2 and -98.66 Kcal/mol, -97.01 Kcal/mol for series 3, providing good insights to understand the structural features responsible for the microbial activity of these molecules.

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Wang resin catalyzed green synthesis of 1,8-dioxo-octahydroxanthene derivatives and their *in silico/in vitro* evaluation against SIRT1

Matta Manikanttha [a], K. Deepti [a] ✉, Mandava Bhuvan Tej [b], A. Gopi Reddy [c], Ravikumar Kapavarapu [d], M.V. Basaveswara Rao [e] ✉, Manojit Pal [f] ✉

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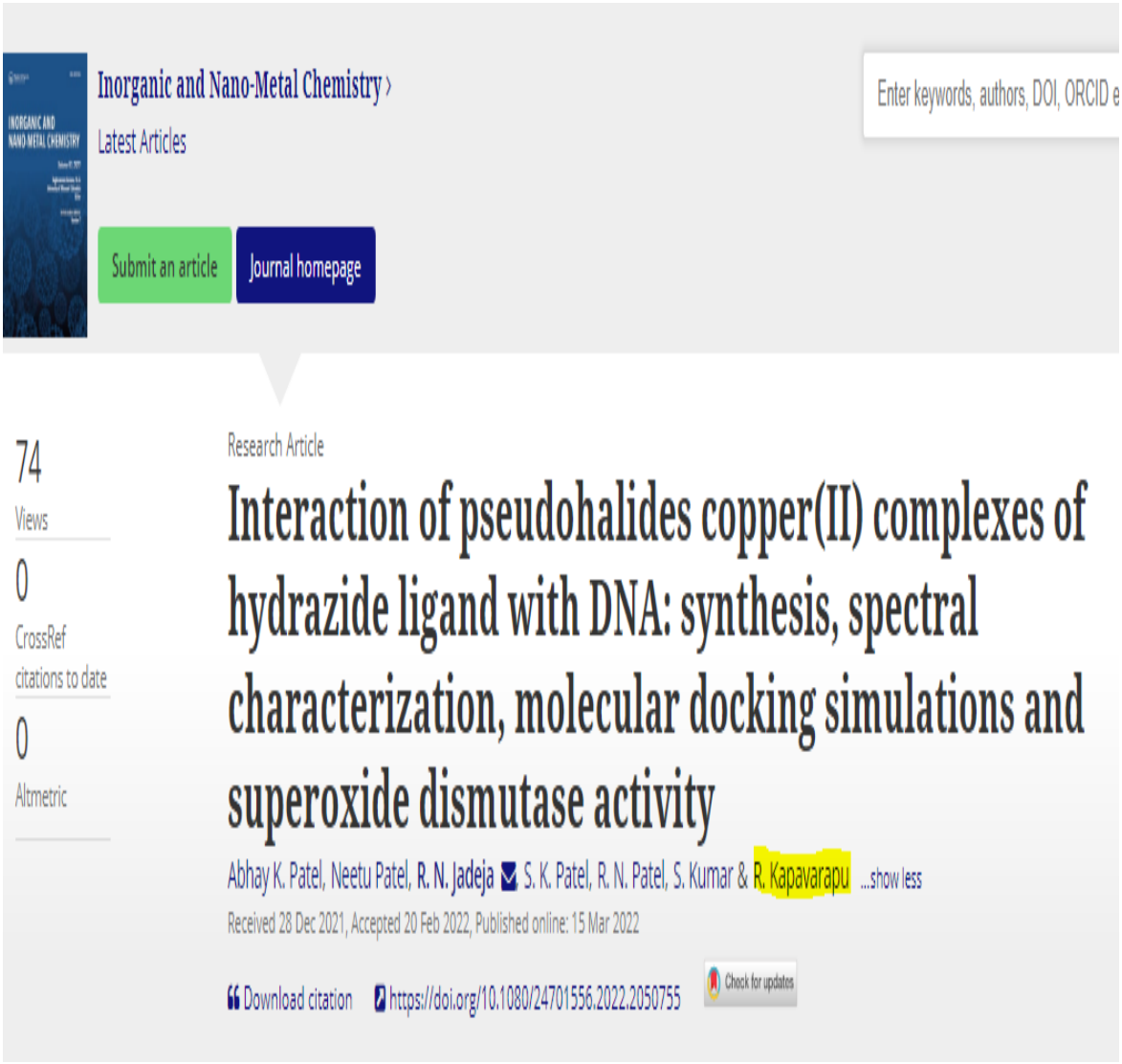

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Sonochemical Synthesis and *In Silico* Evaluation of Imidazo[1,2-*a*]Pyridine Derivatives as Potential Inhibitors of Sirtuins

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