IN-SILICO DRUG DESIGN

Samyakt Jain, Ankit Jain

IPS Academy College of Pharmacy, Indore
samyakt41199@gmail.com, Contact No.9111405252

Abstract: Absorption, distribution, metabolism, excretion, and toxicity (ADME/T) models using In-silico (computer-aided molecular design) have been adopted by an increasing number of pharmaceutical researchers to create effective drugs. We anticipate being able to clearly describe the creation of in silico models for physicochemical qualities, ADME properties, and toxicity assessment while highlighting modeling techniques, applications in drug discovery, and potential benefits and downsides Rational drug design strategies are used to explain how therapeutic molecules that bind to a target location (such as a cellular protein or nucleic acid) are created. . A strategy for identifying lead molecules for additional research that involves determining a compound's drug ability based on a detailed analysis of its medicinal properties. Quantitative structure-activity relationship (QSAR), docking of molecular structures, virtual high-throughput screening, and other approaches are also used in silico drug creation. A target-to-hit and hit-to-lead strategy is utilized to find leads. This disconnect between chemical optimization and ADME/T screening has led to the rejection of numerous candidate medications with high in-vitro efficacy due to their poor drug ability. These issues thus impede the evaluation of the drug's in-vivo efficacy and safety and cause a delay in the research and development process. Early evaluation of compound drug ability will be crucial for increasing R&D productivity and efficiency. The in-silico drug design research using the rational drug technique is inefficient for following investigations because it takes a long time and necessitates several animal tests. Design prefers the novel approach for further drug research because in-silico approaches have been extremely helpful in determining targets and drug prediction.

Keywords: In-silico drug design, Modeling, Rational Drug Design, In-vitro, Absorption, Protein, Drug molecules, Potential.

A Comprehensive review on Herbal hand washes and their benefits

A Sanjeeva Kumar, B Udayasree*, P Bhavana, S Harshitha, P Rajesh, R. Chandrasekhar, Dr. M. Niranjan Babu

Department of Pharmacognosy, Seven Hills College of Pharmacy [A], Venkatramapuram, Ramachandrapuram (Mandal), Tirupati - 517 561, Andhra Pradesh, India
avvarisanjeev@gmail.com, *Contact No.+919441538714*

Abstract: Herbal hand wash is important because it offers a natural and chemical-free way to cleanse hands. It often contains plant-based ingredients with antibacterial properties, which can help kill germs while being gentle on the skin. Additionally, herbal hand washes may have soothing and moisturizing effects, making them a healthier choice for frequent handwashing, promoting hygiene without harsh chemicals. Commonly used plants in hand wash: Aloe vera, neem, tulsi, guava, mentha, Jasmine, Hibiscus, Mimosa pudica, papaya, turmeric, cinnamon, rosemary, eucalyptus, tea tree, Sandal wood, Lemon. Marketed herbal hand washes includes Khadi naturals® which contains sandal wood extract, aloe & lemon, Soul flower® which contains Aloe vera & neem, Jooves® which contains Tulsi, Aloevera & Ginger, Himalaya hand wash® which contains aloe vera & tulsi, Axiom herbal hand wash® which contains neem & aloe vera, Raythe® Eco Trade Pvt. which contains soap nut, neem, tulsi & haridra extract, Arogya herbal hand wash® which contains aloe vera, tulsi, neem & lemon peel and Bio hygiene® which contains lavender flowers, leaves & aloe vera gel. Herbal hand washes are always provided us a way forward to have eco friendly with lesser side effects. In this way, herbal hand wash provides the eco friendly anti microbial action on the hand with minimal or no damage.

Keywords: Herbal hand wash, Anti microbial activity, Medicinal plants, Traditional medicine

Herbal shampoos and their unparallel benefits to mankind

A Sanjeeva Kumar, K Likhitha Reddy*, M Lokeswari, T Bhakthi, N Anil Kumar, P Mohitha, Dr. M. Niranjan Babu

Department of Pharmacognosy, Seven Hills College of Pharmacy [A], Venkatramapuram, Ramachandrapuram (Mandal), Tirupati - 517 561, Andhra Pradesh, India.
avvarisanjeev@gmail.com, +919441538714

Abstract: The most popular type of hair treatment is shampooing. Natural shampoo by having a combination and both organic and natural ingredients stimulates the hair growth of new hair by stimulating the hair follicles while keeping the environment around the follicles clear. It is purpose to remove accumulated sebum, scalp debris and hair grooming treatment residues from the hair. Commonly used plants in herbal shampoos are:Amla, Soap nut, Neem, Aloe vera, Hibiscus, Reetha, Curry leaves, Tulasi, Henna leaves, Bhringraj, Onion, Rose oil, Lemon grass oil. Some of the known marketed herbal shampoos are: Indhulekha antidandruff shampoo® –Amla, Rosemary oil, Mint, Orange oil, Lemon grass oil, Dill. (Herbal concepts health care Pvt. Ltd), Keshking antidandruff shampoo® Haritaki, Bibhitaka, Amla, Aloevera, Lodhra, Tulasi, Methi , Bhringraj, Neem, Shikakai, Manjistha, Brahmi, Jatamansi, Badari, Henna, Nagakesara, Mandukparni, Goksura, Lemon, Rosemary, Karanja.(Ultra beauty care Pvt. Ltd) , Ayush antidandruff shmpoo® Amla, Tulasi, Shikakai, Henna, Neem, Rosemary.(Hindusthan Uni lever Pvt. Ltd), ManMatters®-Caffeine, Argan oil, Biotin, Menthol (Mosaic wellness Pvt. Ltd) and Dabur Vatika herbal shampoo®- Shikakai, Henna, Almond, Amla, Reetha. Commercialization of the prepared shampoo is always advisable but it do carry its specific draw backs which are to be addressed correctly before making it a commercialised product

Keywords: Herbal shampoo, Hair growth, Dandruff, Lice, Medicinal plants

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Organoid Intelligence (OI)

Reshma Parveen Shaik

Maharajah's College Of Pharmacy, Phoolbaugh, Vizianagram - 535002
shaik.reshmaparveen2004@gmail.com, Contact No. +91-9392070359

Abstract: OI is the latest multidisciplinary field that works predominantly in developing the biological computing system by culturing the stem cells of brain and develop then into brain organoids. Organoids were used for drug testing & others. Recently organoids are used in replicating cognitive capacity of human brain. Experiments are done organoids to know the effects of medicine and other substances on organoids and to learn the early stages of neuronal degradation and ways to treat them and find new ways of treating Parkinson and Alzheimer disorders. Now OI are used as biological computers to understand cognitive thinking. The human brain can perform parallel and sequential processing whereas computers can sequential processing only. Human brains have the capacity of storing 2500TB of data which is quite a lot for normal computers for processing. The brain can process the complex data within seconds while the super computers take minutes to process the data. OI is more energy efficient as compared with super computers commercial interest in organoid is increased along with the ethical issues, limitations, regulations on it. OI is used as an alternative to AI so it can better understand biological intelligence. Researchers are planning to combine brain organoids with computing methods to create Bio-computers. Organoids are grown on electrodes to understand neuronal activity and novel treatment of diseases.

Keywords: Organoids, Alzheimer, Cognitive Thinking, Bio-Computers, Sequential Processing, Biological Intelligence

Role of Regenerative Medicine in Treatment of COVID-19 Diseases

Mahesh Barai

RIMT University College of Pharmacy, Mandi Gobindgarh
maheshbarai560@gmail.com, Contact no: 7068415782

Abstract: COVID-19, caused by the severe acute respiratory syndrome coronavirus (SARS-CoV-2), has resulted in a tragic global death toll exceeding 8 million individuals. In the absence of definitive pharmaceutical interventions or vaccines, the exploration of regenerative medicine as a therapeutic approach has gained prominence. This investigative pursuit encompasses the utilization of growth factors, stem cells, tissue engineering, and other regenerative modalities with the aim of mitigating pulmonary complications, bolstering immune responses, and enhancing the prospects of recovery in COVID-19 patients. Given the rapid human-to-human transmission and relatively elevated fatality rate associated with this novel coronavirus malady, COVID-19 has garnered widespread global attention. Ongoing research endeavors seek to ascertain the optimal therapeutic strategies for managing this condition. Regenerative medicine offers an array of cellular and tissue-based therapeutic products, including exosomes, stem cell therapy, natural killer (NK) cell therapy, chimeric antigen receptor (CAR) T cell therapy, and tissue-engineered products, as potential interventions. Studies have consistently highlighted the heightened susceptibility of elderly individuals and those with underlying comorbidities to SARS-CoV-2 infection, often resulting in severe clinical manifestations. The primary objective of this article is to underscore the absence of a definitive curative treatment for COVID-19 to date, while emphasizing the potential of regenerative medicine approaches for addressing this disease.

Keywords: COVID-19, Regenerative medicine, Natural Killer Cells, Coronavirus, Cell Therapy

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Challenges and future trends of lipid nanoparticles in cosmetics and dermal drug delivery

Ayisha Siddiqkha A

Faculty of Pharmacy, Bharath Institute of Higher Education and Research, Tamil Nadu, India
kayishasiddiqkha@gmail.com, Contact no: 8667868027

Abstract: Lipid nanoparticles are creative warship orders grown a suggestion of choice to usual tools in the way that emulsions, liposomes and polymeric nanoparticles. Solid lipid nanoparticles (SLN) and the freshest nanostructured lipid warships (NLC) show main benefits for dermal request of cosmetic and pharmaceuticals.Lipid nanoparticles are intelligentto reinforce drug seepage into the skin, admitting raised address to the skin and therefore growing situation adeptness and lowering the integral incorporation of drugs and beautifying actives. The complete biodegradation of lipid nanoparticles and their biocompatible synthetic type have ensured bureaucracy the title of 'Nano secure one who carries or transmits something.' SLN and NLC show a new mechanics stage, that has existed consumed for one beautifying and drug manufacturing,that will open new channels for persuasive restricted transfer of elements Lipid nanoparticles have arose as a hopeful taxi for cosmetic and dermal drug transmittal, contribution a answer to reinforce the bioavailability and strength of alive compounds. This abstract confers the challenges and future styles guide the request of lipid nanoparticles in these fields. Challenges contain the need for optimizing expression methods, guaranteeing complete cohesion, and giving potential security concerns. Future styles include the investigation often able lipid beginnings, the growth of embodied formulations, and the unification of lipid nanoparticles accompanying leading electronics to a degree Nano sensors and machine intelligence-compelled skin reasoning. Understanding these challenges and flows is alive for controlling the thorough potential of lipid nanoparticles in cosmetic and dermal drug child birth, that can transform skincare and healing approaches.

Keywords: Lipid nanoparticles, Targeted Skin Therapeutics, Encapsulation Efficacy, Skin barrier, Dermal cosmetics.

Virtual reality against painkillers-An Overview

Dhanusha K, Amirtha Lakshmi.B

Faculty of Pharmacy, Bharath Institute of Higher Education and Research, Tamil Nadu, India
dhanushadiv@gmail.com Contact No. 8939360775

Abstract: Adopting fully immersive virtual environments and experiences to manage and alleviate pain, frequently in place of or in addition to conventional painkiller drugs, is known as using virtual reality (VR) as a tool against painkillers. Since virtual reality (VR) is not a medication-based method of treating pain, it does not require the use of conventional pharmacological painkillers. Since atleast1993, when the Medical Virtual Reality programme at the Institute for Creative Technologies at the University of Southern California proposed employing VR to treat post-traumatic stress disorder(PTSD),there has been virtual reality treatment. Virtual reality applications have been shown in numerous research over the past 20 years to offer potential as effective analgesics. Research have shown that the combination of audio hypnosis and VR therapy reduced pain by 57% more than either treatment did on its own. A healthcare provider should decide which drug, if any, is best for the patient based on their unique needs and medical status. Virtual reality (VR) interventions can be used in a variety of ways to manage pain, either in place of or in addition to traditional painkillers. These include immersive VR, distraction VR, exposure therapy VR, physical therapy VR, cognitive behavioural therapy VR, mindfulness VR, and biofeedback VR. There has been a mixed record of success for the numerous virtual reality systems that have been built and studied, ranging in price from low-tech to high-tech. These systems vary from non-immersive 2D VR systems that are used without headgear to fully immersive VR systems with multimodal stimuli.

Keywords: Lipid nanoparticles, Targeted Skin Therapeutics, Encapsulation Efficacy, Skinbarrier, Dermal cosmetics.

E-POSTERS

IN-SILICO DRUG DESIGN

Samyakt Jain, Ankit Jain

IPS Academy College of Pharmacy, Indore
samyakt41199@gmail.com, Contact No.9111405252

Introduction

- Structure-based drug design (SBDD) or in-silico drug design approaches were initiated in the mid 1980s and the first successful applications were reported in the early 1990s.
- A recent study evaluating the link between 60 marketed drugs and their initial leads reported that 11 of the 60 drugs were developed using structure-based design.
- SBDD has become an integral part of most pharmaceutical and biotechnology discovery efforts and it is the major focus of many academic laboratories.

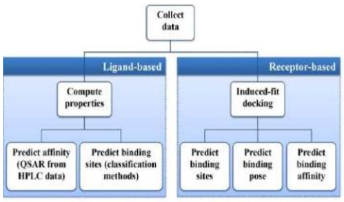
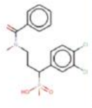


Fig. 1 Schematic of the workflow for the ligand- and receptor-based in silico predicting binding affinity, site, and pose of any userprovided small molecule with HSA.

Fosmidomycin



Disubstituted fosmidomycin analog

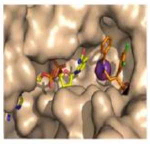


Fig. 2 Representation of a fosmidomycin analog more potent than fosmidomycin in terms of inhibiting *Plasmodium falciparum*

Methods

1. In silico fragment-based drug design

- First introduced in 1981 by Jencks who examined the theoretical benefits of the fragment linking approach.
- introduces the in silico FBDD approach covering the areas of protein structure, protein homology modeling, fragment library construction, binding site identification and druggability, and recent computational approaches to fragment sampling and molecule building to develop hits and leads.
- Advances in high-throughput screening (HTS) facilitated testing these large libraries to identify hits against targets of biological interest with good success.

Other methods also used In-silico

- Ligand-based methods for protein target prediction
- In silico target prediction based on single structures
- Target prediction based on data mining methods
- Chemogenomic approaches

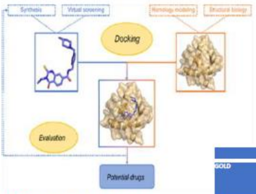


Fig 3 : Summary FBDD approach

Result

- The Novartis group recently validated this model by reporting that hit rates for fragment screens are typically 10 -- 1000 times higher than corresponding HTS screens.
- By in silico FBDD is that computational affinity is not limited by experimental detection limits. This allows inclusion of fragments that are even smaller than 100 Daltons and are less complex, further increasing the chemical space to be interrogated by in silico fragment methods

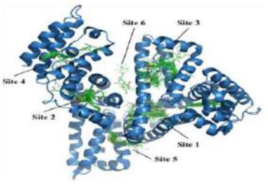


Fig 4 Superimposition of all of the publically available crystal structures of HSA presented, Six drug-binding sites are shown

	Sections	Type of modeling	License	Reference
GOLD	Molecular docking and quantum mechanics, a combined mechanistic tool, Modeling ligand–protein interactions in drug design, Solvent effect as an important parameter	Protein–ligand	Commercial	Verdonk et al[5]
Gaussian (ONIOM)	Molecular docking and quantum mechanics, a combined mechanistic tool	QM/MM	Commercial	Gaussian[6]
AUTODOCK	Modeling ligand–protein interactions in drug design, Solvent effect as an important parameter	Protein–ligand	Open	Morris et al[7]
GLIDE	Modeling ligand–protein interactions in drug design, Solvent effect as an important parameter	Protein–ligand	Commercial	Friesner et al[8]
RosettaDock	Biological complexes and quaternary structures, the protein–protein docking approach	Protein–protein	Open	Lyskov and Gray[9]
pyDOCK	Biological complexes and quaternary structures, the protein–protein docking approach	Protein–protein	Open	Jimenez-Garcia et al[10]
AquaSol	Solvent effect as an important parameter	Solvent effect	Open	Koehl and Delarue[11]

Table: 1the modeling programs listed in this review

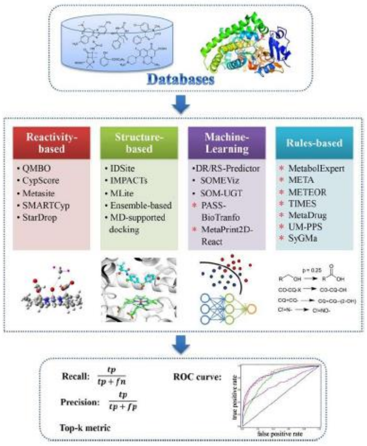


Fig 5 Modelling approaches of some representative models for SOM and metabolite prediction. Models for SOM prediction are labelled as '•', and models for metabolite prediction are labelled with

Conclusion

- In-silico FBDD include binding site identification, targeting druggability characterization, building molecules from fragments to generate leads and carrying out lead optimization.
- Future research will try to improve ligand binding affinity prediction by better accounting for protein flexibility and solvation effects