

Webinar on Nanomedicine: Nanotechnology and Pharmaceutics

March 07, 2022

Scientific Tracks & Abstracts



Sessions

Pharmacy | Toxicology | Pharmacology

Session Introduction

Title: Working goal of Brazilein sappan wood as a candidate for SARS-coV-2 antiviral drug against spike (S) glycoprotein, papain-like protease and main protease: In silico study

Dwi Krihariyani, Surabaya Health Polytechnic, Indonesia

Title: Our experience in treatment with Theresienöl®

Vania Anastasova, Medical University Plovdiv, Bulgaria

Title: Development of a novel filtered-based pharmacophore for the identification of human equilibrative nucleoside transporter 1 inhibitors

Azza Ramadan, Al Ain University, UAE

Title: A Cross-sectional survey: Knowledge, attitudes, and practices of self-medication in medical and pharmacy students

Razan Alduraibi, Qassim University, KSA

Working goal of Brazilein sappan wood as a candidate for SARS-coV-2 antiviral drug against spike (S) glycoprotein, papain-like protease, and main protease: In silico study

Dwi Krihariyani

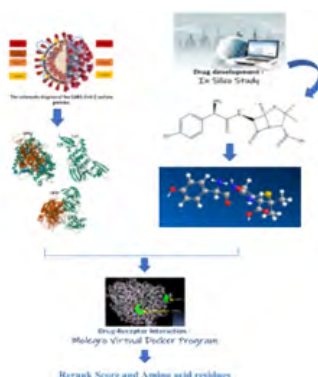
Surabaya Health Polytechnic, Indonesia

Statement of the Problem: SARS-CoV-2 antiviral medicines that can decrease virus attachment, replication, and transcription in the human body are expected to be developed from Brazilein sappan wood. Brazilein has potential as an immunomodulator, has favorable pharmacokinetic properties, and generates relatively low toxicity, according to earlier studies employed in silico tests. Corona viruses connect to ACE2 on human host cells with Spike (S) glycoprotein and then employ Main Protease (MPro) and Papain-like protease (PLpro) to start their life cycle and impair the host response. Using the comparative medicine hydroxychloroquine, the goal of this work was to predict in silico the target of sappan wood brazilein as a candidate for SARS-CoV-2 antiviral treatments against S, PLpro, and MPro proteins.

Methodology & Theoretical Orientation: An in silico test was performed by docking using the Molegro Virtual Docker computer application. The goal of the in silico study is to use a computer to predict the physical chemical properties of chemicals (absorption, distribution, metabolism, and excretion = ADME), as well as their toxicity and biological activity against the target receptor. The bond energy of the docking results between the ligands on the target receptor was compared for data analysis. The lower the ligand's binding energy with the target receptor, the more stable the connection established, and thus the compound's biological activity can be predicted.

Findings: On the Spike (S) glycoprotein target, brazilein offers lower energy than the ligand but greater than hydroxychloroquine, while brazilein provides higher energy than the ligand and hydroxychloroquine on the Papain-like protease and Main protease targets.

Conclusion & Significance: The in silico test revealed that sappan wood brazilein was a viable SARS-CoV-2 therapeutic candidate with stable binding and greater biological activity against S protein than PLpro and Mpro proteins.



Biography

Dwi Krihariyani is a medical laboratory technology lecturer at Surabaya Health Polytechnic who is also interested in health microbiology. My research group and I are currently working on developing Covid-19 antibodies based on pathotype analysis and cloning of the SARS-CoV-2 specific gene, which will be used to generate rapid diagnostic tests.

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Our experience in treatment with Theresienöl®

Vania Nikolaeva Anastasova

Medical University Plovdiv, Bulgaria

Theresienöl® is a traditional Austrian natural product. The family recipe of the product is passed down through the generations. Our experience include treatment of trophic wounds, burns, vulvar leukoplakia, postpartum perineal tear, scar treatment. Theresienöl® contains plant and animal extracts of a 100% natural origin, grown in Tyrol, Austria. Its components act as α -blockers, anti-inflammatory, regenerating and soothing effects on the injuring tissue. The results are very encouraging.

The treatment of trophic wounds is successful in alleviating inflammation, pain, itching and discomfort associated with wound care, thus providing an optimal opportunity for the wound to heal sufficiently and quickly without reported sideeffects.

During the study Facial Burns and Theresienöl® we established significant reduction in the post-traumatic edema, erythema, low tension in the facial area and very good penetration of the oil in the eschars and better esthetic results. After eschars elimination we observe re-epidermalization tissue and no pigmentation as a complication.

It is noteworthy that after Theresienöl® use all patients with vulvar itching reported for no side effects and recurrence of symptoms after the end of treatment were observed during the follow-up period.

In postpartum perineal tear the primary outcome was reducing severity or lacking of some short-term complications, defined as lack of wound dehiscence and hematoma and reducing pain, swelling and redness in this area in the study groups of women over a period of 10 days.

After a series of procedures, we got excellent results with reducing the scar size, pigmentation, pain and itching. Our results show that high-intensity focused ultrasound thermotherapy in combination with Theresienöl® for treatment of pathological scars is a non-invasive method of treatment with excellent results in both aesthetic and functional aspects. In addition, the psycho-emotional and psychological status is very good. Based on this evidence, we believe that outcomes following treatment with Theresienöl® are very good.



Figure 1

Biography

Vania Anastasova works at Department of Burns, Plastic, Reconstructive and Aesthetic Surgery since 2005 year. She has experience in burn treatment, wound healing and reconstructive technics. She is Associated Professor since 2011 years. It this model after years of experience in research, evaluation, teaching and administration both in hospital and education institutions. She is General Researcher in University Project about the effect of Theresienöl®.

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Development of a novel filtered-based pharmacophore for the identification of human equilibrative nucleoside transporter 1 inhibitors

Azza Ramadan

Al Ain University, UAE

Statement of the Problem: The human equilibrative nucleoside transporters (hENTs) are important transporters that allow nucleosides and nucleobases permeation into the cell. hENT 1 is a promising target against heart and Huntington’s diseases as its inhibition mediates cardiac- and neural protection effects, respectively. However, the current hENT1 inhibitors have significant off-target effects and poor pharmacological profile. Hence there is a need for new novel inhibitors.

Methodology: Therefore, we developed a computational protocol for developing ligand-based pharmacophores that identify and select inhibitors of hENT1 in an efficient and specific manner. To examine the efficacy of the pharmacophore and its application later on in the drug discovery of new hENT1 inhibitors, we used this pharmacophore as a filter prior to a small-scale virtual screening (VS) of a drug-like ligand library. The library consisted of 5000 compounds; 56 of which were known hENT1 inhibitors.

Findings: First, several pharmacophores were created using a set of known inhibitors. Among the several created pharmacophores, the best inhibitor pharmacophore exhibited high selectivity and specificity rates of 92% and 88%, respectively. Furthermore, another pharmacophore was validated for the oppositely acting type of the hENT1 molecules (i.e. permeants) to act as an extra refinement step in our search for hENT1 inhibitors. Interestingly, employing the inhibitor pharmacophore as a filter-in along with the permeant pharmacophore as a filter-out resulted in up to twofold enhancement of docking-based virtual screening results (see Table 1).

Conclusion & Significance: This in silico approach can prove very useful in the discovery of new cardio- and neuroprotective hENT1 inhibitors.

Table 1. Retrieved rate of hENT1 inhibitors at various portions of the sorted docked ligands from filter-based and non-filtered-based virtual screening

Output percentage of the top-ranked docked 5000-ligand library	The rate of retrieved inhibitors		
	No-filter	One filter	Two filters
1	12.5	19.6	21.27
3	17.8	35.29	34.04
5	26.78	49.02	48.93
10	42.85	80.39	80.85
20	57.14	98.04	100

Biography

Azza Ramadan is a molecular biologist and currently an Assistant Professor at Al Ain University in the United Arab Emirates. She obtained her PhD from the University of Toronto in Canada with a specialization in biomedical sciences. Among her areas of research, is investigating the role of the human equilibration nucleoside membrane transporter hENT1 in cardio and neuroprotection. Her research interest stems from her work during her graduate studies that shed light on ENT1 central role in purinergic signalling in the cardiovascular system. Her research was supervised by the internationally renowned expert in membrane transport proteins, Prof Imogen Coe.

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A cross-sectional survey: Knowledge, attitudes, and practices of self-medication in medical and pharmacy students

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Qassim university, KSA

Background: Self-Medication is common practice worldwide in both developed and developing countries. Self-Medication is referred as self consumption of medication without consulting a physician for either diagnosis or treatment. This study aimed to assess the knowledge, attitudes and practices toward self-medication among medical and pharmacy students.

Methods: This cross-sectional study was conducted among medical and pharmacy students in Qassim university, Buraydah, Saudi Arabia, during the period 2020-2021. Multistage random sampling technique was used to recruit students. The data were collected through questionnaire.

Results: Three hundred and sixteen of 316 students were recruited. This study showed that the majority (94.6%) of students had good knowledge of self-medication. Additionally, the following characteristics were significantly associated with good knowledge: being female, and Pharmacy students. Overall mean score for the attitudes towards self-medication shows that 58.4% of the total sample had high agreements towards the questions of the attitudes toward self-medication. More than half (63.9%) of the students reported that they practice self- medication in the last 6 months. Pain killers was the most common medication used for self- medication by the majority of the students (88.29%).

Conclusions: In conclusion, students' knowledge of self-medication appears to be good and significantly high among pharmacy students in comparison to medical students. As well self-medication was highly practiced among the students. Therefore, medical and pharmacy students should be viewed as important contributors to the public health care system, and future health professionals should be properly educated on good pharmacy practice and responsible self-medication.

Biography

I am an undergraduate medical student at Qassim university. I grew up in a family how knows the meaning of being a doctor, as 5th of my elder saplings are already graduated from medical college and are involved in a different specialty. Being a physician was a natural progression for me. I'm an active young doctor who is willing to be keen and confident enough to provide the best medical help to the patients and community.

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