



PHARMACEUTICAL SCIENCES IN A TRANSFORMING WORLD:
RESILIENCE AND STRENGTHENING BY MULTI-DISCIPLINARY STRATEGIES

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ABSTRACTS BOOK

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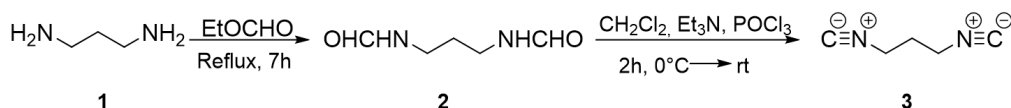
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PO1 - SYNTHESIS OF 1,3-DIISOCYANOPROPANE AND APPLICATION IN UGI FOUR-COMPONENT REACTIONSMike Gustavo Coelho (Brazil)¹; Paulo Marcos Donate (Brazil)¹

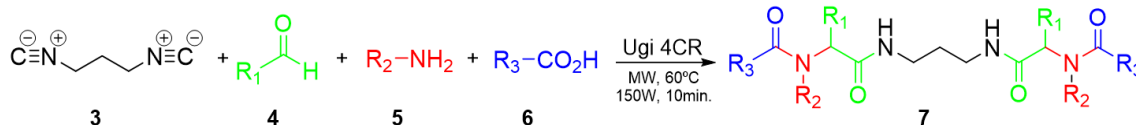
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Keywords: multicomponent reactions, isocyanides, Ugi-4CR.

The Ugi reaction is a multicomponent process that is widely applied in the pharmaceutical industry to prepare libraries of compounds. This reaction is very useful to produce peptoid-like backbones that occur in many biologically important heterocycles. Isocyanide is a functional group possessing dual nucleophilic and electrophilic character that has been used as an important reactant in multicomponent reactions for the syntheses of a variety of functionalized peptides. A molecule with two isocyanide groups represents an attractive starting material for many applications, as for example, in new drugs discovery. Therefore, in this work, the synthesis of 1,3-diisocyanopropane (Scheme 1) was performed for application in Ugi four-component reactions (Ugi 4CR) (Scheme 2).



Scheme 1: Two-step synthetic route to 1,3-diisocyanopropane.



Scheme 2: Reaction of the diisocyanide 3 in Ugi 4CR.

The products were analyzed by NMR. The obtained spectra were consistent with the structures of the desired products.

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Obrecht, R.; Herrmann, R.; Ugi, I. Isocyanide synthesis with phosphoryl chloride and diisopropylamine. *Synthesis* (1985): 400–402.

PO2 - PREPARATION AND PHYSICOCHEMICAL CHARACTERIZATION OF CATIONIC LIPOSOMES FOR DRUG DELIVERY IN THE INFLAMED INTESTINAL EPITHELIUM

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Keywords: cationic liposomes, drug delivery, thermodynamic stability.

Inflammatory bowel diseases (IBD) are chronic diseases that have unsatisfactory treatments, and for this reason, new treatments have been investigated [1]. The objective of this work was to prepare and characterize cationic liposomes (CLs) of L- α -phosphatidylcholine egg yolk (EPC), 1,2-dioleoyl-*sn*-glycero-3-phosphoethanolamine (DOPE) and 1,2-dioleoyl-3-trimethylammonium-propane (DOTAP) (CLs-EPC/DOPE/DOTAP), which in the future will be combined with natural polymers for drug delivery in the inflamed intestinal epithelium. The CLs-EPC/DOPE/DOTAP were prepared based on the methodology of Gasperini et al. (2015) [2] with three extrusion

cycles at 65 ± 2 °C on a polycarbonate membrane (\varnothing 100 nm) and then, characterized by dynamic light scattering (DLS) and phase analysis light scattering (PALS). The liposomes had a hydrodynamic size of 64.68 ± 1.40 nm, a polydispersity index of 0.305 ± 0.004 and a zeta potential of $+43.57 \pm 4.86$ mV. The results indicated that the CLs-EPC/DOPE/DOTAP presented nanometric particles, medium polydispersity and thermodynamic stability.

Acknowledgements: PROSUC/CAPES; INCT-NanoFarma; FAPESP (Process number: 2014/50928-2); CNPq (Process number: 465687/2014-8); University of Sorocaba (UNISO).

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PO3 - MOLECULAR MODELING STUDIES AND SYNTHESIS OF ARILFURANS AS POTENTIAL INHIBITORS OF THE FAAH ENZYME

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Keywords: FAAH inhibitors, endocannabinoid system, molecular docking, chemical synthesis.

The endocannabinoid system is involved in several pathophysiological functions, such as neural modulation and anti-inflammatory activity. The main ligand of this system, anandamide (AEA), has shown important analgesic activity against painful trauma. Nevertheless, AEA's half-life is short, determined by its degradation mediated by fatty acid amide hydrolase (FAAH). Thus, our group research proposed 44 arylfuran analogues of a known FAAH inhibitor (OL-135) and evaluate their *in silico* affinity by molecular docking technique. The docking protocol was performed using a crystalized humanized rFAAH ligand-protein complex, employing the ChemScore as scoring function. As result, the calculated interactions pattern of the analogues corroborated experimental binding modes of known FAAH inhibitors and 7 of them has shown interaction scores higher than the crystallographic ligand itself. Two of the highest score ligands (1 and 2) had already been synthesized and characterized as well as will have their analgesic activity evaluated by neuropathic pain models

PO4 - PATIENT SAFETY AND HIGH-ALERT MEDICATIONS: ANALYSIS OF REPORTED INCIDENTS AT A PUBLIC TEACHING HOSPITAL

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Keywords: High-alert medications, Patient Safety, Pharmacovigilance

A subgroup of medicines deserves special attention because they present a higher risk or probability of causing severe harm to the patient when used incorrectly, being called High-Alert Medications. This study aimed to analyze the reports of incidents related to this subgroup distributed at a teaching hospital in the interior of São Paulo. This study is descriptive and retrospective, where the analysis was performed based on notifications of medicines made during the years 2009 to 2018, present in the institution's database. Of the total number of reports, 301 were related to high-alert medications. The notifications were of technical complaints 31.56%, adverse drug reactions 31.56%, therapeutic inefficacy 32.22%, and other reports 4.65%. It was concluded that there were an expressive number of notifications and the need to adopt strategies to minimize the damage caused by the inappropriate use of these medicines.

PO5 - MANGO PEEL AND PULP AS INDUCERS OF CARBOHYDRATE-DEGRADING ENZYMES IN T. HARZIANUM

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Keywords: enzymes, mangifera, *Trichoderma*.

Insoluble polysaccharides (IP) are a key virulence factor for dental biofilms. Nevertheless, enzymes from the fungus *Trichoderma harzianum* can convert this polymer into soluble sugars, which could be an innovative strategy to disassembly biofilms and control dental caries. This study aimed to evaluate the induction of IP-degrading enzymes using Peel and Pulp mango as carbon sources. Crude Peel and Pulp (Total, Precipitated, and Filtered) were added into culture mediums with (F+) and without the fungus (F-, control group). Culture medium with fungus alone acted as an internal control. After incubation for 192h, reducing sugars (RS) were quantified by the Ferricyanide method. The results were analyzed by the ANOVA test followed by Tukey or Bonferroni post-test. All groups were different compared to the internal control group ($p < 0.001$), however, only Precipitated Pulp presented higher RS for F+, suggesting that this fraction could be a feasible inducer of IP-degrading enzymes in *T. harzianum*.

PO6 - INTERVENTIONS TO REDUCE THE PRESCRIPTION OF POTENTIALLY INAPPROPRIATE MEDICATIONS COSTS

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Keywords: Economic Evaluation, Health Interventions, Inappropriate Prescribing.

Introduction: Interventions have been evaluated to reduce prescription of potentially inappropriate medications for elderly (PIM) and health-care costs. **Objective:** Identify interventions and cost components of PIM prescriptions. **Methods:** A systematic review was conducted in PubMed and Scopus (October 2020). **Results:** Eleven studies

published between 2014 and 2020 were identified. The studies assessed direct medical costs and four reported the perspective (payer). The interventions conducted were medication review (n=8); PIM deprescription (n=2); and medication review with PIM deprescription (n=1). The cost components evaluated in the interventions were costs of drug acquisition (n=6), use of health service (n=2), saving in drug acquisition (n=2) and cost-effectiveness of intervention (n=1). All interventions reduced the number of PIM prescribed, in three studies the interventions were not cost-effectiveness, that is, interventions were not effective in reduce associated costs. Conclusion: Our data suggests that the identified interventions were effective in reducing PIM prescription.

Acknowledgements: São Paulo Research Foundation (FAPESP) [grant number 2019/01565-8; 2018/07501-9] and National Council for Scientific and Technological Development (CNPq) [grant number 459461/2014-1]. This study was financed in part by the Coordination for the Improvement of Higher Education Personnel - Brazil (CAPES) - Finance Code 001.

PO7 - THERE IS NO ADDITIVE INTERACTION BETWEEN THE RS1799983 GENETIC VARIANT AND THE USE OF LOW-DOSE ASPIRIN IN THE RISK OF GASTROINTESTINAL BLEEDING

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Keywords: Drug-related side effects and adverse reactions, Genetic polymorphism, Patient Safety.

Introduction: Idiosyncratic responses in low-dose aspirin (LDA) users have been described, especially upper gastrointestinal bleeding (UGIB) due to the presence of genetic variants. **Objective:** It was intended to assess additive interaction between the rs1799983 variant (gene *NOS3*) and LDA use in the occurrence of UGIB. **Methods:** Case-control study including 200 cases with UGIB and 706 controls was conducted in a Brazilian hospital. Synergism index (S) and Relative Excess Risk due to Interaction (RERI) were estimated through regression models adjusted for history of ulcer, bleeding, and dyspepsia; cardiovascular disease; cholesterol; *Helicobacter pylori* infection; nonsteroidal anti-inflammatory drugs and anticoagulants use; and alcohol and tobacco ingestion. **Results:** Although an increased UGIB risk was identified in LDA users carriers of rs1799983 genetic variation (OR: 4.63; CI95%: 2.16-9.92), no additive interaction was identified [RERI: 1.93 (CI95%: -1.45-5.31)/ S: 0.49 (CI95%: 0.10-2.49)]. **Conclusion:** Our data evidence no joint biological action between rs1799983 genetic variation and LDA use on UGIB risk.

Acknowledgment: São Paulo Research Foundation (FAPESP) [2017/24193-4; 2018/07501-9] and Conselho Nacional para o Desenvolvimento Científico e Tecnológico (CNPq) [401060/2014-4]. This study was financed in part by the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior - Brasil (CAPES) - Finance Code 001.

PO8 - *PHYSALIS ANGULATA* L. ENDOPHYTIC FUNGI EXTRACT AGAINST *ESCHERICHIA COLI*

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Keywords: Physalis angulata, endophytic fungi, Escherichia coli.

Endophytic fungi are known to develop inside plant tissues without harming the host. Higher plants can harbor different species of endophytic fungi, although some are more easily colonized. The isolation of endophytic fungi of *Physalis angulata* was carried out by washing with sterile distilled water and cutting the leaf and root fragments. Immersion in 70% alcohol, 2.5% and 5% sodium hypochlorite and sterile distilled water was performed. The fragments were seeded on Potato Dextrose Agar medium with penicillin G and streptomycin sulfate and incubated at 28 °C for up to 60 days. Endophytes named as R3M2.5 (from the root) and F45B (from the leaf) were selected. The development of experiments against *Escherichia coli* was based on the guidelines of Standard M7-A10 according to CLSI. The extract of the endophytic R3M2.5 showed the lowest MIC against *E. coli* while the F45B remained without activity up to the highest concentration analyzed.

PO9 - COVID-19 ANTIGEN POINT-OF-CARE TESTS PERFORMANCE COMPARISON

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Keywords: COVID-19, Antigen, Point-of-care testing

COVID-19 antigen (Ag) point-of-care tests (POCT) are relatively inexpensive immunoassays used to identify a current SARS-CoV-2 infection. Along with other strategies, serial antigen testing every three days or so can identify early SARS-CoV-2 infection and reduce transmission. Efficient monitoring depends on the frequency and speed of testing, reporting and interventions, but the test performance also contributes to it. In this study, we compared the performance characteristics, sensitivity and specificity, of eight COVID-19 Ag POCT. Results from the Hilab COVID-19 Ag POCT clinical evaluation assay were compared to data sheet information from seven other commercial tests: Abbott Panbio COVID-19 Ag Rapid Test, RapiGEN BIOCREDIT COVID-19 Ag, Healgen Coronavirus Ag Rapid Test, Coris BioConcept COVID-19 Ag Respi-Strip, R-Biopharm RIDA QUICK SARS-CoV-2 Antigen, Nal von minden NADAL COVID-19 Ag Test and Roche SARS-CoV-2 Rapid Antigen Test. The Hilab test presented a very high performance in this comparative analysis, with sensitivity and specificity values greater than 99%.

PO10 - INNOVATIVE TRANSFERSOMES FOR THE TRANSDERMAL NANODELIVERY OF IBUPROFEN

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Keywords: ibuprofen, transfersomes, transdermal delivery.

The chronic use of Ibuprofen *per os* is greatly hampered by the occurrence of gastrointestinal toxicity. Its transdermal delivery may be a promising alternative, but the epidermal barrier greatly blocks the skin permeation of drugs (1). The use of transfersomes as nanodelivery systems seems to be a valuable strategy for transdermal applications (2).

Hence, this work aimed at developing an ibuprofen-loaded transfersomal formulation using a Box-Behnken design strategy, as previously reported (3). This quality-by-design approach was successfully implemented, as the optimized formulation displayed a suitable size for cutaneous applications (< 300 nm), a homogeneous size distribution (polydispersity index < 0.3), and favorable drug loading. The transfersomal formulation was also stable under refrigerated conditions for at least 1 month and it was further characterized by Fourier-transform infrared spectroscopy and *in vitro* permeation studies.

Altogether, these data indicate that transfersomes may be interesting nanosystems to improve the transdermal delivery of ibuprofen.

Acknowledgements: This work was funded by national funds through Fundação para a Ciência e a Tecnologia (FCT), under the UIDB/04567/2020 and UIDP/04567/2020 projects to CBIOS.

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PO11 - SYNTHESIS AND ANTIOXIDANT ACTIVITY EVALUATION OF DERIVATIVES AND ANALOGUES OF CANNABIDIOL

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Keywords: cannabidiol, antioxidant, medicinal chemistry.

Cannabis is a genus of plants widely used through the millennia for ritualistic, hedonistic and medicinal purposes and presents hundreds of phytocompounds, with cannabidiol (CBD) being one of the most relevant. Despite having several biological activities, such as analgesic, anti-inflammatory, anticonvulsant, antioxidant and neuroprotective, it has unfavorable pharmacokinetic properties. To investigate the antioxidant effects and improve activity and pharmacokinetic parameters of CBD, alkyl, aldehyde and amino derivatives and analogues of CBD and olivetol, its bioprecursor, were synthesized. Three different antioxidant assays, FRAP, DDPH and ABTS+, were performed to evaluate the antioxidant potential of the synthesized compounds. On FRAP assay, CBD derivative MPP CBD CL displayed the highest activity (80.68 μ MTE/mM of sample). Additionally, the same compound presented the highest activity on DPPH and ABTS (49.18%AAT and 50.69%AAT, respectively). CBD presented solid results on FRAP, DPPH and ABTS (129.99 μ MTE/mM of sample, 18.24%AAT and 41.22%AAT, respectively). Additionally, Trolox was used to create a calibration curve to FRAP, and as positive control to DPPH and ABTS (24.82%AAT and 98.93%AAT, respectively). Nevertheless, CBD derivatives and analogues have presented satisfying activity, further experiments are necessary to confirm their activity *in vivo*.

PO12 - MEAN ABSOLUTE PERCENTAGE ERROR (MAPE) AS A RELIABLE TOOL FOR ASSESSING REACTION TIME IN IMMUNOCHROMATOGRAPHY TESTS

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Keywords: validation, precision, stability.

In the clinical laboratory, stability testing is an important step to ensure the test performance is stable to the end user. The most traditional approaches (e.g. accelerated and real-time stability) focus on evaluating the overall shelf-life of reagent kits in storage and shipping conditions. On the other hand, these are usually inadequate for estimating the optimal reaction time range, which is essential for in-house validation. Here, we show an accessible

approach to evaluate the accuracy over time in Thyroid-Stimulating Hormone (TSH) quantification. Controls were read in triplicate for 15 min at different time intervals, including the optimum reaction time indicated by the supplier (around 10 min). MAPE was estimated by comparing the concentration from precision studies with each time interval, and a MAPE >20% indicated instability. MAPE shows up as a reliable approach for estimating result stability in the clinical laboratory.

PO13 - QUANTIFYING VARIATION IN THE CLINICAL LABORATORY FOR IMPROVING EXTERNAL QUALITY CONTROL

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Keywords: proficiency, quality control, clinical agreement.

External quality control (or proficiency testing) is an important tool for quality assurance, especially for ISO accreditation, since it helps laboratories in identifying trends and deviations in analytical measurements thus enabling corrective actions to be taken. However, a deeper analysis for accuracy of quantitative data is not always possible once acceptable range is often overestimated. Consequently, comparing average laboratories performance – within or outside the average range – can be misleading in defining the analytical performance of a laboratory. Here, we take proficiency testing further by evaluating total agreement (for quantitative and qualitative assays) and variation between analytical runs (Total Error %) to assess the reliability of quantitative results for HbA1c, Total Cholesterol (CHOL) and Triglycerides (TG). The proposed method is a potential tool for taking proficiency testing to the next level thus aiding in continuous improvement of processes.

PO14 - CONNECTING PHARMACY STUDENTS AND REAL-LIFE CLINICAL SERVICES: THE REFERENCE CENTER FOR DRUG INFORMATION (CRIMED)

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Keywords: pharmaceutical education, correct use of medication, clinical services

Drug Information Centers (DIC) are operational units that provide objective clinical and chemical data of drugs, being strategic for supporting prescription, dispensing and drug administration. In 2020, the Reference Center for Drug Information (CRIMED) was created as a research and extension project to connect pharmacy students with real-life situations of healthcare market through pharmacists. Beyond the provision of strategic drug information, CRIMED supports resolution of clinical cases presented by professionals registered as partners of the center. Thus, a technical guide with 18 parameters was created to summarize the most relevant drug information, in order to help pharmacists and students with rapid and updated data. So far, CRIMED supports pharmacists in hospitals, pharmacies and drugstores in Minas Gerais and Ceará states. Students' knowledge of pharmacology has improved, and employment opportunities have increased, as the institutions in partnership are more open to hire the trained students as they graduate.

PO15 - POTENTIAL OF ENZYME PRODUCTION BY *TRICHODERMA HARZIANUM* GROWN IN MANGO FIBER WASTE

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Keywords: mango, waste, *Trichoderma harzianum*

Mango fiber waste (MFW) is the major by-product of mango juice industry and the high cost of its proper disposal has been the focus of researches on ways to make them useful. This work aimed to evaluate the potential of MFW as an inducer of enzymes of biotechnological interest by *Trichoderma harzianum*. Reactivated fungus was incubated in culture medium containing yeast extract and Khanna salts in presence (MFW+) or absence (MFW-) of fiber extracted from Tommy Atkins' mango. After incubation for 192h, proteins and reducing sugars (RS) were quantified. Data analysis (t-test) showed statistical difference between groups for protein (MFW+: 57.8±4.8; MFW-: 6.1±4.2; p<0.0001) but no for RS (MFW+: 536.7±38.3; MFW-: 481.5±34.0; p=0.1). Although promising, more studies should be carried out to further refine the potential use of MFW as substrate to produce enzymes under a cheap fermentation, reducing problems associated with wastes disposal and contributing to studies in biotechnology.

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PO16 - INSTRUMENTAL MEASUREMENTS AND SENSORY ANALYSIS OF COSMETIC FORMULATIONS WITH ALFALFA AND LENTIL EXTRACTS

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Keywords: texture properties, sensorial properties, mature skin.

The ingredients of cosmetic formulations can influence the stability, sensory properties, and efficacy of the products. In this context, the aim of this study was to evaluate the texture profile by instrumental measurements and sensorial properties of a cosmetic formulation added to alfalfa and lentil extracts. Measurements in terms of

consistency, firmness, cohesiveness, index of viscosity, and work of shear were performed. The results showed that the formulation with or without (vehicle) the extracts presented similar texture parameters, except for the consistency, which presented lower values for the vehicle. In addition, the formulations showed good sensory properties. However, the formulation containing the extracts showed different sensory properties in the parameters touch sensation and skin smoothness. In conclusion, the formulation containing the extracts showed good sensorial and texture properties, which suggest the use of these natural extracts to obtain a formulation with suitable sensory properties according to product's use purpose.

PO17 - SCHISTOSOMA MANSONI INFECTION INFLUENCES EXPLORATORY ACTIVITY OF MALE BALB/C MICES

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Keywords: *Schistosoma mansoni*, Exploratory behavior, nociception, Mice.

Schistosoma mansoni infection may involve the central nervous system and result in abnormal behavior (Fiore et al., 1998; Fidelis et al., 2020). In this study, male Balb/C mice were percutaneously infected with 50 cercariae of *S. mansoni* and evaluated in behavioral tests (Open field, Hole-board, Hot-plate) 2 and 4 weeks after infection. Our findings show significant reductions in exploratory behavior, with decreased head-dipping and frequency of rearing in the Hole-board and Open Field tests, respectively, in weeks 2 and 4 ($p < 0,01$). However, there were no differences in nociception in the Hot-plate test. The results indicate that infection by *S. mansoni* impairs the levels of attention and motivation associated with exploratory behavior, as well as the performance of vertical movements, which may be associated with the production of cytokines and growth factors as result of the immune response to the infection (Coyle, 2013).

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PO18 - CHEMICAL COMPOSITION AND TRYPANOCIDAL ACTIVITY OF *PIPER MARGINATUM* ESSENTIAL OIL COLLECTED IN ITACOATIARA, AMAZONAS

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Keywords: Chagas disease, *Piper*, volatile compounds.

The Piperaceae family comprises 5 genera and approximately 2.000 species, of which 140-300 species are found in the Amazon. The *Trypanosoma cruzi* parasite is the causative agent of Chagas Disease and represents an important public health problem in endemic regions. The objective of this work was to evaluate the chemical composition and trypanocidal activity of the essential oil from fresh leaves of *Piper marginatum* (PM). Plant material was collected in the city of Itacoatiara-AM for extraction of essential oil by hydrodistillation using a Clevenger apparatus. The essential oil showed a yield of 0.13%. Being mostly constituted by (*Z*)- β -ocimene and (*E*)- β -ocimene. PM showed moderate activity on the trypomastigote forms of *T. cruzi* with an IC₅₀ of 69.5 $\mu\text{g/mL}^3$ (Table 1). As well as previous studies showed inhibition of the growth of epimastigote forms of *T. cruzi* for the *P. marginatum* essential oil. The continuation of this study may provide support for the development of therapeutic alternatives to combat the parasite.

PO19 - COMPATIBILITY STUDY OF AVOBENZONE WITH EXCIPIENTS COMMONLY USED IN THE DEVELOPMENT OF NANOSTRUCTURED LIPID CARRIERS

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Keywords: Avobenzone, preformulation, sunscreen, nanotechnology

Photoprotection has become an essential topic in daily life due to the resulting increase of skin cancer incidences. Nanostructured Lipid Carriers (NLC's) have been described in scientific reports as carriers for various cosmetics actives. It has been found that these lipid nanoparticles act as physical sunscreens on their own. The aim of this work was to evaluate Avobenzone's compatibility against 5 oils, commonly used in CLN preparation. Initially the chromatography method was validated following RDC 166/2017, according to the parameters of linearity, precision, accuracy, selectivity and detection limits. The Avobenzone's interactions were evaluated by thermogravimetric analysis (TG/DTG/DTA) and FTIR techniques. In TG/DTG/DTA results, is suggestive of non-interaction was observed, while in FTIR chemical interaction with Caprylic/capric triglyceride was shown. Therefore, further investigation is needed to define interactions and compatibility of oils with AVB.

PO20 - VALIDATION OF A POINT-OF-CARE TESTING FOR DENGUE NS1 ANTIGEN, A BRAZILIAN ENDEMIC DISEASE

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Keywords: validation, dengue, point-of-care-testing.

Dengue is a mosquito-borne viral infection widespread throughout the tropics. According to WHO, 1,465,243 dengue cases were reported in Brazil in 2020, with an incidence rate of 702.77 cases per 100,000 population and 554 deaths. Numbers are often under-reported, since the majority of cases are asymptomatic, mild or self-managed, similar to other febrile illnesses. Dengue NS1 antigenemia is a risk factor associated with severe disease. Therefore, it is important to provide a reliable point-of-care testing (POCT) for screening dengue at the onset of symptoms, especially far from urban centers. In this study we compared the Hilab Dengue NS1 Antigen POCT to the gold-standard methodology for dengue NS1 diagnosis. Our POCT showed a Kappa index of 1.00 (95% CI: 0.86-1.00) and relative sensitivity (95% CI: 90%-100%) and specificity (95% CI: 95%-100%) above 99%, suggesting a high agreement between methods, validating the efficiency of the test.

PO21 - RHEOLOGICAL ANALYSIS AS A PREFORMULATION TOOL TO FDM 3D PRINTING OF DRUG PRODUCTS

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Keywords: Additive manufacturing; Hot-melt extrusion; Viscoelasticity.

The study aimed to assess the utility of rheology to guide the development of medicines by FDM 3D printing. In this work, polymers used in FDM printing — high impact polystyrene, polylactic acid, polyvinyl alcohol, and common plasticizers — mineral oil, triethyl citrate, and glycerol respectively, were evaluated using the thermolabile model drug isoniazid. A temperature ramp from 20 to 200 °C was used to determine the glass transition, complex viscosity, storage, loss, and complex moduli. The results showed that the heating of the samples simulating the FDM 3D printing process could produce changes in their viscoelastic behavior, even when no degradation processes occurred. Moreover, chemical incompatibilities may damage the polymer chain's deformation capacity impairing printing, whereas the correct polymer:drug:plasticizer combination reduces complex viscosity, improving matrix printability. Thus, this work shows the importance of assessing the viscoelastic behavior of pharmaceuticals to support the rational choice of compatible components for FDM printing.

PO22 - EFFECT OF A PROBIOTIC DRINK ON WEIGHT CONTROL OF MICE FED A HIGH-FAT DIET

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Keywords: obesity, probiotic, intestinal microbiota

The aim of the study was to verify whether the daily intake of a probiotic drink (*Enterococcus faecium* CRL 183, *Lactobacillus helveticus* 416 and *Bifidobacterium longum* ATCC 15707) based on aqueous soybean extract can modulate the composition of the microbiota and control the weight gain of mice fed a high-fat diet. The weight, daily feed intake and the composition of the fecal microbiota by the determination of *Lactobacillus* spp., *Bifidobacterium* spp., *Enterobacteriaceae*, *Clostridium* spp. and *Enterococcus* spp. was monitored throughout the 70 days protocol. The weight of the animals receiving the probiotic drink remained without significant changes until 35 days of study and the microbiota showed a reduction in the *Enterobacteriaceae* population and an increase in beneficial microorganisms (*Bifidobacterium* spp. and *Lactobacillus* spp.). Therefore, the daily intake of the probiotic product showed beneficial effects for the control of obesity, positively modulating the microbiota of the animals.

PO23 - DEVELOPMENT OF POLYURETHANE IMPLANTS CONTAINING ANTI-TOXOPLASMA AND ANTI-INFLAMMATORY DRUGS TO TREAT THE OCULAR TOXOPLASMOSIS

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Keywords: polyurethane implants, ocular toxoplasmosis, ocular implants.

Ocular toxoplasmosis is an infectious disease that compromises the eye. Retinal lesions lead to inflammatory processes, and both may lead to the reduction of visual acuity and blindness. Drugs do not penetrate, in therapeutic doses, into the posterior segment of the eye. To improve the treatment of ocular toxoplasmosis, implants based on polyurethane (7 g), trimethoprim (200 µg), sulfamethoxazole (1 g), and dexamethasone acetate (400 µg) were developed to improve the conventional therapy. Implants released therapeutic doses of the drugs for 90 days. *In vitro* biocompatibility of implants and possible degradation products from polyurethane was evaluated by using ARPE-19 cells; and the cellular viability in direct contact with these substances was evidenced. In addition, they reduced the number of *Toxoplasma gondii* in infected ARPE-19 cells. In conclusion, implants based on polyurethane, trimethoprim, sulfamethoxazole, and dexamethasone acetate may represent a therapeutic alternative to treat the ocular toxoplasmosis.

PO24 - IDENTIFICATION OF POTENTIAL HDAC3 INHIBITORS FOR THE TREATMENT OF ALZHEIMER'S DISEASE

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Keywords: epigenetic regulation, in silico, natural products

Alzheimer's disease (AD) is a neurodegenerative disorder associated with aging. Studies have indicated the roles of epigenetics in its pathogenesis. Epigenetic marks such as acetylation of histones, show variations in AD patients. Such post-translational modifications are regulated by histone acetyltransferases (HATs) that relax chromatin and histones deacetylases (HDACs) which condense the chromatin. Experiments indicate that overexpression of HDAC3 compromises gene expression, leading to loss of synaptic plasticity and memory in AD. In order to identify potential inhibitors of this target, we used structure-based virtual screening (SBVS) technique considering a subset of 80763 natural products of ZINC15. The structure of HDAC3 was downloaded from Protein Data Bank (PDB). The Autodock Vina software was used for the study of the VSBE, where three sequential steps were carried out to filter potential inhibitors against HDAC3. The RGFP966 inhibitor was used as a control. Thus, it was possible to select 148 compounds with score ≤ -9.0 Kcal.mol⁻¹. The ADME properties were evaluated using the SwissADME software, where it was possible to identify 2 potential inhibitors with desirable pharmacokinetics. Our results suggest that compounds derived from 1-benzylpyrrolidine-2,5-dione may possess characteristics favorable pharmacological to inhibit HDAC3.

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PO25 - EFFECT OF OIL FROM BARU ALMONDS (*DIPTERYX ALATA* VOG.) IN A TYPE 2 DIABETES MELLITUS WISTAR RAT MODEL

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Keywords: Diabetes Mellitus, Wistar Rats, Functional Food, Dipteryx

Diabetes Mellitus is a chronic metabolic disorder characterized by hyperglycemia. Oil from baru seeds is a source of monounsaturated fatty acids. Oleic acid stimulates glucagon-like peptide-1 secretion (GLP-1), inducing insulin secretion. This study aimed to assess the insulinotropic effect of oil from baru almonds. Male Wistar rats were

feed with high fat diet for 4 weeks, followed by a 35mg/kg-1 streptozotocin injection. Baru oil was administrated to control and diabetic groups, at the doses of 1g/kg, 1,5g/kg, 2g/kg. Insulin and glucose tolerance tests were performed. Glucose, lipid and liver function biomarkers were assessed. Histological and histomorphometric analysis of pancreas and liver were also performed. Baru oil improved glucose and insulin tolerance in diabetic rats ($p < 0,01$), but not the fasting glucose levels, nor fructosamine levels. Diabetic animals treated with 2g/kg showed Langerhans islets area increased, evidences of hepatocitotoxicity and insulin resistance. Oleic acid in baru oil might affects insulin receptor sensitivity

PO26 - PBPK MODELING TO PREDICT CARVEDILOL EXPOSURE IN PATIENTS UNDERGOING ROUX-EN-Y GASTRIC BYPASS SURGERY

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Keywords: carvedilol, PBPK, bariatric surgery, RYGB.

Anatomical and physiological changes after Roux-en-Y gastric bypass (RYGB) for obese patients may alter the drug's pharmacokinetics (PK). This study aimed to evaluate carvedilol PK before and after RYGB and to validate a physiologically based pharmacokinetic (PBPK) model to predict the oral bioavailability of carvedilol after RYGB. The full PBPK model for carvedilol was implemented using Simcyp[®] (v20). Observed data from healthy volunteers, obese patients and post-RYGB were compared to predicted results from PBPK simulations. The model successfully predicted the AUC, C_{max} and T_{max} (with predicted/observed ratio within 2-fold) in healthy volunteers' data from 16 published datasets and morbidly obese patients ($n=2$; pred/obs ratios of AUC^{0-inf} , C_{max} , T_{max} of 0.86, 0.71, and 0.63, respectively). However, an overprediction of carvedilol plasma concentrations was observed in the current PBPK model for post-RYGB patients ($n=2$; pred/obs ratios of AUC^{0-inf} , C_{max} , T_{max} were 2.51, 6.33, and 1.56, respectively). Clinical data from obese and post-RYGB patients is currently being assessed to optimize the PBPK models in the RYGB population.

PO27 - EFFECT OF POTENTIALLY PROBIOTIC COMMENSAL STRAINS ON MOUSE-INDUCED COLITIS

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Keywords: colitis, probiotic, microbiota

Despite probiotic microorganisms helping to reduce symptoms and increase remission periods of colitis, their beneficial effects are often divergent, evidencing the strain-specific effect and a possible influence of the resilience of the intestinal microbiota. The aim of this study was to evaluate the effect of daily intake of commensal bacterial strains, isolated from the gut microbiota, on DSS-induced colitis in mice. During the experimental period (14 days), the disease activity index (DAI), composition of the fecal microbiota and histological changes in the colon

were monitored. The group treated with commensal strains showed a reduction in colitis symptoms (DAI), less histological changes in the colon and an increase in the population of Bifidobacterium spp. which is important in maintaining intestinal homeostasis. The results indicate that the use of strains isolated from the indigenous microbiota is a promising approach to controlling symptoms and reducing the risk of colitis.

PO28 - SIMULATED TRAINING AND LEARNING APPROACH FOR A COMPOUNDING PHARMACY

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Keywords: Compounding pharmacists, Active teaching-learning methodologies, Simulation, Pharmaceutical education.

Pharmacy undergraduate curriculum requires the use of active teaching-learning methodologies. This work aimed to use simulation to integrate pharmaceutical production theory with the work routine of compounding pharmacies. Thus, handling a medicine from a real prescription was simulated in a laboratory divided into six workstations: I. attend the patient and order the medicine; II. generate a production order and carry out the pharmaceutical evaluation of the prescription; III. identify, define and calculate raw materials concentration, correction and dilution factors; IV. Handling of medicine and choice of packaging; V. Inspection of final product, packaging, labeling and VI. Drugs dispensing and pharmaceutical counseling. The students performed the role of pharmacist or patient in each workstation. These activities provided an overview of the pharmaceutical compounding process and connected theory to practice.

PO29 - ELECTROSPUN NANOFIBER AS A DELIVERY SYSTEM FOR VITAMIN C

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Keywords: ascorbic acid, delivery system, electrospinning, nanofiber.

Vitamin C or ascorbic acid (AA) is a potent antioxidant extensively used as a cosmetic active due to its antioxidant, antiaging and antipigmentary properties. However, this ingredient is easily degraded when exposed to light, high temperatures and water, hampering its application in conventional cosmetic forms. This research aimed to develop electrospun nanofibers as a new material for AA skin deliver. To produce the material, a polymeric solution containing ethyl cellulose (EC), ethanol, acetone and AA was electrospun, and an EC/AA nanofiber was successfully developed. Through scanning electron microscopy, it was observed the formation of interconnected fibers, shaping a three-dimensional structure that has large surface area with the fiber's average diameter of $226 \pm 53\text{nm}$ (Fig.1).Electrospun nanofiber is an interesting material for skin delivery system.

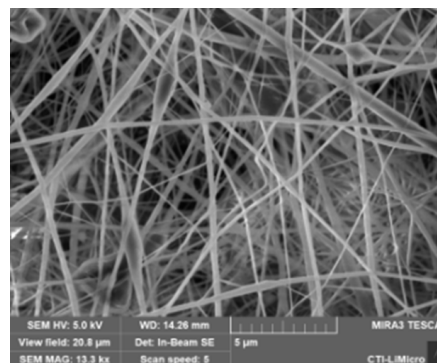


Fig.: SEM of ethyl cellulose nanofiber with ascorbic acid.

Incorporating active ingredients, such as AA, into the nanofibers could improve the performance of cosmetics, since studies shown its ability to effectively transport ingredients to the skin, protecting them from oxidative processes. We believe that this material is very innovative and has the potential to enhance the benefits of cosmetic actives, reducing treatment time and increasing product stability.

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PO30 - PRODUCTION AND STERILIZATION OF POLYMERIC MEMBRANES

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Keywords: Polymers, eletrospinning, scaffolds.

Studies aimed at tissue engineering have gained prominence in recent decades, having as one of the main objectives, the development of materials that simulate biological tissues, which can be applied in prostheses, grafts, skin, among others. The biomaterials used for this purpose are obtained from synthetic or natural polymers. Polymers have stood out in the production of polymeric scaffolds and one of the most used ways to obtain these devices is electrospinning. The main polymers most used are: poly (glycolic acid) (PGA), poly (lactic acid) (PLA), Polyhydroxybutyrate (PHB), polycaprolactone (PCL) and poly (vinyl alcohol) (PVA) and their copolymers.

The purpose of this study is to manufacture Core-Shell (PVA) and (PLA) membranes, verify their barrier function or selectivity, as well as establish material sterilization tests, considering the implementation of bioassays.

PO31 - IDENTIFICATION OF THE MAIN BARRIERS FOR MONITORING CARDIOTOXICITY IN ONCOHEMATOLOGIC PATIENTS TREATED AT AN UNIVERSITY HOSPITAL IN THE STATE OF RIO DE JANEIRO

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Keywords: cardiotoxicity, university hospital, monitoring.

Cardiotoxicity (CTX) is one of the most serious complications of oncohematological treatment, being often responsible for the worsening of the clinical picture and the interruption of therapy. The objective of this study was to identify the main barriers for monitoring CTX in oncohematological patients treated in a university hospital. A quantitative research was carried out, in which an online questionnaire was applied to a group of specialists formed by the hospital's health professionals to answer questions regarding the main barriers to monitoring the CTX. The project was approved by the Research Ethics Committee. The results showed that all respondents consider that there are barriers and the main one is the absence of internal protocols (60%) and the difficulty of communication between sectors (40%). Results indicate the need to develop clinical protocols and greater integration, which is already being carried out at the hospital, through meetings between sectors to discuss this topic.

Acknowledgements: This work was supported by Fundação de Amparo à Pesquisa do Estado do Rio de Janeiro (FAPERJ).

PO32 - THE INFLUENCE OF ALCOHOL GEL POLYMERS ON THE STABILITY TEXTURE PROPERTIES, SENSORY AND HYDROLIPIDIC CHARACTERISTICS OF THE SKIN

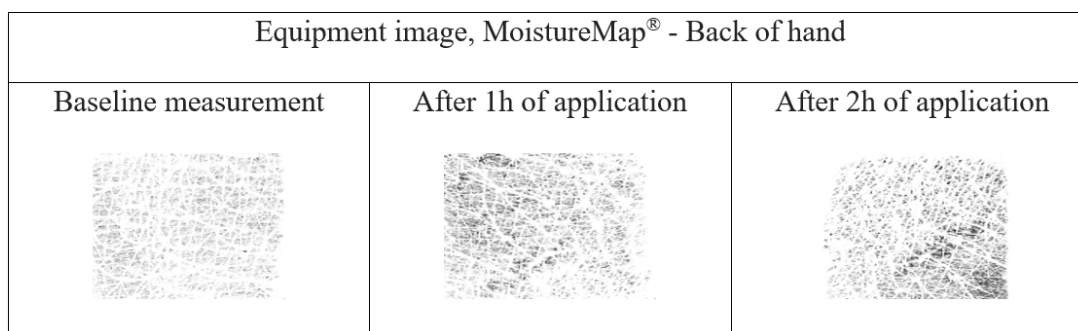
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Keywords: Physical-mechanical profile, clinical efficacy, alcohol-gel

The skin, being the largest organ in the body, performs different functions to maintain the body's homeostasis and protect it against possible pathogens (1, 2). In addition, it has been proven that excessive sanitation, which increased significantly during the pandemic, can trigger mechanisms that damage the skin and its barrier function (3), so the present study aimed at the elaboration of hydrating alcohol gel formulations as well as the evaluation of its characteristics. Formulations were developed with acrylate polymers added with D-Panthenol, known to increase skin hydration and contribute to the barrier function (4). Thus, they were evaluated for their physical-mechanical characteristics, with the use of Texturometer and Rheometer, sensory, and clinical efficacy with the use of imaging equipment, Visioscan[®] and MoistureMap[®], transepidermal water loss, Tewameter[®], and of the hydration level, Corneometer[®], to prove the improvement in the skin's barrier function.



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PO33 - CLINICAL EFFICACY OF A COSMETIC FORMULATION CONTAINING OLIVE EXTRACT BY REFLECTANCE CONFOCAL MICROSCOPY

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Keywords: Skin photoaging, olive fruit extract, cosmetics, RCM.

Considering that the ingredients from natural sources have been very used for the skin care, the aim of this study was to evaluate the clinical efficacy of a cosmetic formulation containing olive extract standardized in hydroxytyrosol in the improving of photoaging skin. Before and after a 42-day period of application of the formulation with olive extract, measurements in terms of epidermis layer thickness and number of hyperreflective pixels were performed by Reflectance Confocal Microscopy (RCM). The results showed a significant increase in the granular layer thickness after a 42-day period of treatment with the formulation under study when compared with baseline values, which suggests an improvement of cell renewal. In addition, a significant decrease in the number of hyperreflective pixels as well as a reduction in the basal layer brightness after the treatment was observed, suggesting an improvement of skin hyperpigmentation pattern. The study subjects also perceived the efficacy of the formulation under study once they reported an improvement of skin luminosity after the period of treatment. In conclusion, the proposed formulation based on olive extract was effective in the improving of skin photoaging.

PO34 - POLYMERIC MEMBRANES FOR GUIDED BONE REGENERATION IN DENTISTRY

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Keywords: Core-Shell, Guided Bone Regeneration, scaffolds.

Oral health is an important factor for people's quality of life, because individuals with compromised oral health can have their self-esteem affected, as they can present problems in their speech, swallowing and/or chewing. Among the diseases that affect oral health are periodontitis, an inflammatory disease that leads to eventual tooth loss. When this happens, it is necessary to perform a local regeneration for future placement of dental implants. Among the most used techniques to achieve this rehabilitation is Guided Bone Regeneration (GBR), which uses barrier membranes that provide space for bone filling to occur. The objectives of this study are the incorporation of growth factors in Core-Shell membranes and their efficiency as a cellular scaffolds.

PO35 - DOXYCYCLINE IN AQUACULTURE: STUDIES OF DRUG INCORPORATION IN THE FEED

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Keywords: Doxycycline, aquaculture, medicated feed.

Doxycycline is a broad-spectrum antimicrobial and its effectiveness is recognized for the treatment of bacterial diseases that affect fish species. Its use in fish farming is not yet regulated in Brazil, although it is approved in other countries. Methods of incorporation of the drug in the feed using gelatin and using ethylcellulose were developed aiming at a homogeneous process, avoiding the risk of drug leaching from the feed to water. The methods showed incorporation efficiency of ~70% and resulted in a homogeneous medicated feed (CV<2%) (n=9). In the leaching tests, within 15 minutes, <5.1% of the doxycycline was leached into water. An extraction procedure was developed, optimized and validated to determine the concentration of doxycycline in the feed. The developed methods showed extraction efficiency of 95% (CV 5,8%), linearity (r>0.99), precision (CV<3.4%) and recovery factor (>97.4 and <102). Analyzes were performed using liquid chromatography associated with tandem mass spectrometry.

PO36 - STUDY OF ENVIRONMENTAL EXPOSURE MODELS TO ASSESS THE IMPACT OF COSMETICS INGREDIENTS DISPOSED ON DOWN-THE-DRAIN

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Keywords: environmental exposure models, risk assessment, personal care products.

Every year a high amount and variety of raw materials and personal care products are discharged in wastewater treatment facilities. However, to determine the real environmental exposure is a challenge, because it depends on multiple factors, such as substance quantity used by exposed population and place dilution factor in which the substance was discharged. In this context, a theoretical and detailed study of three screening model tools,

which use standardized data to analyse and perform a comprehensive evaluation that could be extrapolated for the Brazilian scenario was performed. The analyses performed by each tool were tabulated as well as all necessary inputs and outputs for the assessment process. According to the obtained results, it was possible to compare, choose and evaluate the feasibility of better environmental model tools for the implementation and assessment of the environmental safety of cosmetics ingredients in Brazil, in order to contribute to the decision-making process.

PO37 - THIN LAYER CHROMATOGRAPHY ANALYSIS OF PHARMACEUTICAL FORM OF *Achyrocline satureioides* PRODUCED AT THE “FARMÁCIA DA NATUREZA DA TERRA DE ISMAEL”

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Keywords: *Achyrocline satureioides*, thin layer chromatography, luteolin, quercetin.

The identification of chemical markers is a fundamental requirement to guarantee the quality of the herbal medicinal products and patient safety. The objective of this work was to perform the quality control of *A. satureioides* tincture, through chemical identification of quercetin and luteolin flavonoids, using the thin layer chromatography (TLC) technique. Aliquots of flavonoid standards and *A. satureioides* tincture were spotted separately on TLC plate (cellulose with fluorescence) using chloroform: acetic acid: water (50:45:5) as mobile phase. After development, the plate was air-dried at room temperature and the spots were visualized under UV spectrum at 254 and 365 nm before and after spraying the TLC plate with NP/PEG reagent. Afterward, R_f values for the detected spots were calculated. TLC was a highly effective analytical method for characterization of luteolin and quercetin in the analyzed herbal medicinal product, being a cost-effective option for the quality control of *A. satureioides* tincture.

PO38 - IN SILICO EVALUATION OF NATURAL FLAVONOIDS INTERACTION WITH SPECIFIC PROSTATE MEMBRANE ANTIGEN

Leones Fernandes Evangelista (Brazil)¹; Lucas Matheus da Paz (Brazil)¹; Mac Dionys Rodrigues da Costa (Brazil)¹; Igor Moreira de Almeida (Brazil)¹; Mateus Edson da Silva (Brazil)¹; Pedro Nonato da Silva Júnior (Brazil)¹; Emanuel Paula Magalhães (Brazil)¹; Ramon Róseo Paula Pessoa Bezerra de Menezes (Brazil)¹; Alice Maria Costa Martins (Brazil)¹; Tiago Lima Sampaio (Brazil)¹

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Keywords: Prostate cancer, Flavonoids, Molecular Docking

The effectiveness, high toxicity and costs of the current chemotherapy treatments for Prostate cancer (PC) show the importance of new pharmacological tools development, like those employing natural products, as flavonoid, which pharmacological activities are very well known. Then, the present study aimed to evaluate the in silico interaction of flavonoids with the specific prostate membrane antigen (PSMA). Thus, Apigenin (AG), Catechin (CT), Epicatechin (EC), Genistein (GN), Kaempferol (KF), Luteolin (LT), Myricetin (MT), Quercetin (QT) and Silymarin (SM) chemical structures were docked with PSMA protein (PDB: 3D7H) using the SwissDock platform, being evaluated values of binding energy (ΔG – kcal/mol), distances (Å) and binding types. Thereby, EC (-8.9) and SM (-8.6) presented higher values of ΔG . EC, LT and QT presented strong hydrogen bonds interactions. Thus, we reinforce the potential of the present molecules, mainly EC and SM, as promisor pharmacologic tools to treatment of PC. The authors thanks to CNPq and CAPES for their financial support.

PO39 - PHYSIOLOGICALLY BASED PHARMACOKINETIC MODELING OF HIDROXYCHLOROQUINE ENANTIOMERS IN HEALTHY VOLUNTEERS

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Keywords: hydroxychloroquine, enantiomers, PBPK

Hydroxychloroquine (HCQ) is clinically available as a racemic mixture of (-)-*R*-HCQ and (+)-*S*-HCQ. The current work aimed to develop and validate for the first time PBPK models for (-)-*R*-HCQ and (+)-*S*-HCQ. Whole-body PBPK models for (-)-*R*-HCQ and (+)-*S*-HCQ were developed using Simcyp® (v.20). Evaluation of the predictions was based on concentration–time profiles from studies in healthy volunteers after single oral dose of 155 mg *rac*-HCQ. The model successfully predicted area under the curve (AUC), maximum blood concentration (C_{max}) and time to reach C_{max} (T_{max}) in three independent clinical studies.¹⁻³ Mean fold errors (MFE) of predicted/observed AUC, C_{max} and T_{max} varied from 0.88-1.84, 0.64-1.19 and 0.65-1.0 for (-)-*R*-HCQ and 0.61-1.3, 0.58-1.1, and 0.50-0.86 for (+)-*S*-HCQ, respectively. Simulations have shown higher blood exposure for (-)-*R*-HCQ than that of (+)-*S*-HCQ. In conclusion, the developed PBPK model showed accurate predictions of the concentration profiles and pharmacokinetic parameters of HCQ enantiomers in healthy volunteers.

PO40 - PRESERVATIVE EFFICACY TESTING OF COSMETIC FORMULATIONS CONTAINING PRESERVATIVES FROM NATURAL SOURCE

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Keywords: natural preservatives, cosmetics, antimicrobial efficacy, *Xylityl Sesquicaprylate* and *Caprylyl Glycol*

The use of ingredients of natural source is growing in the cosmetic market. In addition, there is a trend for the use of natural preservatives as an alternative to synthetic preservatives. *Xylityl Sesquicaprylate* and *Caprylyl Glycol* can be used as preservatives obtained from natural source in cosmetic formulations. In this context, the aim of this study was to evaluate the antimicrobial efficacy of cosmetic formulations containing *Xylityl Sesquicaprylate* and this in combination with *Caprylyl Glycol*. For the preservative efficacy testing, the following test microorganisms were used: *Staphylococcus aureus* (ATCC 6538), *Pseudomonas aeruginosa* (ATCC 9027), *Escherichia coli* (ATCC 10536) and *Candida albicans* (ATCC 11006). The evaluation of the log reduction of the microorganisms was performed every 7 days during 28 days. The bacteria were grown on Tryptic Soy Agar and the fungus on Sabouraud Dextrose agar. The results showed that both formulations reached the USP standard, with 2 log reductions of all four microorganism in the first 14 days and no log scale increases in the remaining days. In conclusion, the proposed preservatives showed antimicrobial efficacy in the cosmetic formulations under study. Thus, they can be suggested as an alternative in the development of cosmetic formulations based on natural ingredients.

PO41 - INFLUENCE OF A COSMETIC FORMULATION ON NATURAL MOISTURIZING FACTORS (NMF) BY CONFOCAL RAMAN SPECTROSCOPY (CRS)

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Keywords: d-panthenol, lactic acid, moisturizing, skin barrier function.

Topical d-panthenol has been shown to act as a skin moisturizer with barrier-enhancing properties, however, its exact action mechanisms have not been fully elucidated. Thus, the aim of this study was to evaluate the *in vivo* effects of topical d-panthenol on skin's Natural Moisturizing Factors (NMF) by Confocal Raman Spectroscopy (CRS). For this purpose, ten healthy subjects underwent NMF evaluation by a CRS 3510 skin analyser, before and after two hours of applying a cosmetic formulation containing or not (vehicle) 5% d-panthenol. Spectral data were acquired in the fingerprint region obtained from the skin of the anterior forearm, immediately before and 120 minutes after application. Semi-quantitative determination of the NMF, performed using the least square fit of the spectra, pointed to an increase factor of 1.86 for lactic acid relative amounts when compared to the vehicle. Indeed, as a constituent of the alpha-hydroxy acid (AHA) group, lactic acid exhibits cell renewal functions in addition to humectancy. In conclusion, evidence on d-panthenol's effects on NMF contributes to the elucidation of its moisturizing mechanisms and other concurrent biochemical processes.

PO42 - COMPARATIVE EVALUATION OF QUALITY AND IN VITRO PERFORMANCE OF HARD CAPSULES

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Keywords: gelatin capsules, hypromellose capsules, pullulan capsules

The hypromellose (HPMC) and pullulan capsules have excellent properties and are promising as far as regulatory, manufacturing, religious, and dietary issues are concerned. This study aims to develop and evaluate *in vitro* characteristics of formulations containing amoxicillin (as a model drug) in HPMC and pullulan shells compared to conventional hard gelatin capsules. Amoxicillin capsules were produced manually and evaluated for uniformity, disintegration time and *in vitro* dissolution profile (USP I, water at 37°C, 100 rpm). The results demonstrated that owing to their greater water permeability, gelatin capsules disintegrate and drug release much faster than HPMC and pullulan shells.

The results indicated that it is necessary to evaluate the drug characteristics and its therapeutic action time, since the HPMC and pullulan capsules presented an initial release time higher than the gelatin capsules. In addition, it is necessary to evaluate the formulation stability as well as the possible incompatibility between the drug and the materials shell.

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PO43 - STRUCTURAL MODELING OF TMPRSS2 AND MOLECULAR DOCKING WITH CAMOSTAT

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Keywords: SARS-CoV-2, TMPRSS2, Structural bioinformatics.

The TMPRSS2 is an important serine-protease that activates the membrane fusion by the SARS-CoV-2 S protein. Although it is an exciting therapeutic target against COVID-19, there is no experimental molecular structure to explore such molecular interactions. In this study, we modeled the extracellular domains of TMPRSS2 by different strategies using homology modeling and threading, and compared the best models by structural assessment tools. The best model obtained by the threading approach (Figure 1a) was subjected to molecular dynamics simulation (Figure 1b) and evaluated by RMSD, RMSF, and Rg. Camostat, an already approved drug that inhibits SARS-CoV-2 viral entry *in vitro*, was docked in the protease domain after pocket prediction (Figure 1c and d) and the molecular interactions between the target and the ligand were assessed. Such results might help the drug design or repurposing of TMPRSS2 inhibitors and elucidate the roles of TMPRSS2 in viral infections and cancer.

PO44 - NANOSTRUCTURED LIPID CARRIERS FOR NASAL ADMINISTRATION OF DONEPEZIL: IN VITRO RELEASE STUDIES

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Keywords: donepezil, nanostructured lipid carries, nasal administration, *in vitro* release.

Donepezil is used in the Alzheimer's disease by the oral route, but several side effects have been reported. Considering the ability of the nasal route to increase brain bioavailability, we developed nanostructured lipid carriers (NLC) for nasal administration of donepezil employing stearic acid, oleic acid, tween[®] 80, poloxamer 188 and water (30:10:10:10:40, w/v). The *in vitro* release of donepezil from NLC was performed Franz- type diffusion cells. Phosphate buffer (20mM, pH 5), stirred at 300rpm and maintained at 37°C was used as the release medium to assure sink conditions. At predetermined time intervals, aliquots were withdrawn, and the amount of donepezil released was determined by HPLC. The NLC sustained donepezil release according to Higuchi's kinetic ($r=0.9119\pm 0.0192$), releasing 25% in only 0.25h and reaching 56% in 6h. Then, NLC developed for the nasal administration of donepezil may be promising for the treatment of Alzheimer's disease.

PO45 - PRODUCTION OF XYLOOLIGOSACCHARIDES FROM SUGARCANE BAGASSE HEMICELLULOSE BY IMMOBILIZED ENDOXYLANASE FROM *THERMOMYCES LANUGINOSUS*

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Keywords: Xylanase, Fungus, Xylooligosaccharides

This study aimed to evaluate the production of xylo-oligosaccharides from hemicellulose obtained from sugarcane bagasse by the action of immobilized endoxylanase from *Thermomyces lanuginosus*. The maximum immobilization yield of 78.5% with pure endoxylanase (50U) from *T. lanuginosus* was obtained at a concentration of 4% sodium alginate and 300 mM calcium chloride. The immobilized endoxylanase was evaluated for its application in hydrolyzing the hemicellulose from sugarcane bagasse in 50 mM phosphate buffer pH 6.5 at 65 °C under agitation. The hydrolysis of sugarcane bagasse hemicellulose by the immobilized enzyme resulted in the release of 1.75 mg/mL and 1.06 mg/mL of total sugar in the first and second cycle, respectively. Furthermore, the total sugar products obtained after 60 min were short-chain xylooligosaccharides. Thus, the immobilized endoxylanase showed qualities that allow the production of XOS from hemicellulose from an abundant agricultural residue.

Acknowledgements: This work was supported by CAPES and Fundação Araucária.

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PO46 - *IN VITRO* EFFECTIVENESS OF BRAZILIAN GREEN PROPOLIS EXTRACT AS PHOTOSENSITIZER IN PHOTODYNAMIC THERAPY ON *STREPTOCOCCUS MUTANS*

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Keywords: antimicrobial photodynamic therapy, Brazilian green propolis, natural photosensitizer.

Aim: To evaluate *in vitro* the efficacy of two Brazilian green propolis (BGP) extracts against *Streptococcus mutans* in antimicrobial photodynamic therapy (aPDT). **Material and methods:** *S. mutans* ATCC 35688 suspension and biofilms were used. aPDT was carried out in duplicate at 96-well plates containing 50 μ L of *S. mutans* and 50 μ L of BGP extracts individually. The samples were incubated for 5 minutes and irradiated with blue LED (IrradLED® – Biopdi, Sao Carlos, SP, Brazil) for 18 minutes at fractionated mode irradiation. After the irradiation, cell viability in each group (n=10) was assessed by CFU counts. Statistical significance was considered at $\alpha < 0.05$. **Results:** A total microbial reduction (7.86 log CFU/mL) was observed for *S. mutans* suspensions for both BGP extracts. Reductions greater than 3 log CFU/mL were observed for *S. mutans* biofilms. **Conclusion:** Both BGP extracts showed efficacy as photosensitizer on aPDT against *S. mutans*.

PO47 - PHYSIOLOGICALLY BASED PHARMACOKINETIC (PBPK) MODEL TO ASSESS POTENCIAL DISEASE-DRUG-DRUG INTERACTIONS WITH REMDESIVIR

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Keywords: remdesivir, DDI, PBPK

Remdesivir is indicated for COVID-19 in adults and adolescents with pneumonia that require oxygen supplementation. In this study, we aim to use PBPK model to predict disease-drug-drug interactions with remdesivir. Model build was based on data of remdesivir prodrug (GS-5734), and its two metabolites (GS-704277 and GS-441524), which were uploaded into Simcyp[®] simulator (v.20). Evaluation of the model predictions was performed using concentration–time profiles in healthy volunteers treated with intravenous infusion of remdesivir from three clinical studies¹⁻². The model successfully predicted (observed/predicted ratio within 2-fold) the AUC and T_{max} of remdesivir and its metabolites for the dosages of 3 to 225 mg/day (single-dose study), 150 mg/day for 7 days, and 200 mg on day 1, then 100 mg/day for 5 or 10 days (both multiple-dose studies). Overpredictions of the metabolites were observed only for 3 mg. Subsequently, the model predictions will be validated using other clinical studies. PBPK simulations will be applied to evaluate the combined effect of multiple drug-drug interactions and disease-drug interactions with remdesivir.

PO48 - CHEMINFORMATIC ANALYSIS OF SELECTIVITY IN THE ACTIVE SITES OF CYSTEINE PROTEASES FROM THE PAPAINE FAMILY TO DESIGN NOVEL DIPEPTIDYL NITRILE INHIBITORS

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Keywords: cheminformatics, structure-based drug design, molecular interaction field (MIF).

Cysteine proteases are involved in many physiopathological processes in human diseases, targeted by small chemicals in drug discovery & development projects. The enzymes involved in this work belong to the papain family and are therapeutic targets for several pathologies: cruzain from *Trypanosoma cruzi* and human cathepsins: B, L, S (cancer), and K (osteoporosis). The high similarity among the enzymes is a challenge to design selective inhibitors. Therefore, the active sites of the proteins were mapped using molecular interaction fields using *in silico* chemical probes. Principal component analysis was applied in these data to highlight the selective regions, rationalizing the search for chemical groups to design novel dipeptidyl nitrile inhibitors with high potency. These chemicals were docked along with ChEMBL representatives to select the best candidates for synthesis and biochemical assays. This study could guide the selection of building blocks in a hybrid approach joining ligand and structure-based drug designs.

PO49 - HAND CARE FORMULATIONS: STABILITY AND RHEOLOGICAL BEHAVIOR

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Keywords: cosmetics, rheology, hand cream

Nowadays, the consumption of hand care products has been increasing due to the skin dryness caused by the increasing of hand hygienization. Considering that, an ideal hand cream formulation should be flow properties that easy the application, such as a good spreadability and touch sense, the evaluation of rheological behavior is very important to obtain a stable and suitable cosmetic product for the hand care. Thus, the objective of this study was to develop and evaluate the rheological properties of a moisturizing hand cream formulation containing D-Panthenol. The studied formulations, vehicle and formulation containing Panthenol, were stable and showed a pseudoplastic thixotropic rheological behavior. The formulation with panthenol showed higher consistency index when compared to vehicle. In addition, this formulation presented higher tixotropy, which can be correlated with a good spreadability of the formulation during application. Finally, rheological measurements can contribute to predicting the performance of cosmetics on the skin.

PO50 - INFLUENCE OF VEHICLE ON ASCORBYL TETRAISOPALMITATE SKIN PENETRATION: *IN VIVO* EVALUATION BY CONFOCAL RAMAN SPECTROSCOPY

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Keywords: skin penetration profile, cosmetic formulations, vitamin C derivative, Confocal Raman Spectroscopy.

The vehicle composition significantly affects the cutaneous penetration of active ingredients either by altering polarity, molecular partitioning or because of action mechanisms. Confocal Raman Spectroscopy (CRS) is a renowned technique for sensitive and non-destructive analysis of *in vivo* skin penetration. Thus, the aim of this study was to evaluate the *in vivo* skin penetration of ascorbyl tetraispalmitate (ATIP) when vehiculated into two different vehicles, a transdermal and a conventional emulsion. Ten healthy subjects participated in the skin penetration evaluation of ATIP by CRS. Spectral data were acquired from the fingerprint region obtained from the skin of the anterior forearm, immediately before and after 120 and 240 minutes after application. Maximum depth permeated by ATIP in both formulations was 45 μm . Liquid effect and permeation profiles derived with respect to the relative intensities and the 2nd derivative of ATIP at 1708 cm^{-1} showed depth-dependent intensities and increasing slope relative to ATIP vehiculated by the transdermal emulsion at the epidermis. Penetration profiles and semi-quantitative analysis revealed that the active substance was found in different relative amounts at the stratum corneum and epidermis, as per vehicle, pointing out the importance of the choice of vehicle according to product's use purpose.

PO51 - IMPACT OF COVID-19 PANDEMIC ON THE CHANGES OF HAND HYGIENE HABITS AND SELF-CARE WITH HAND AND FACE SKIN

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Keywords: Skin care, hygiene habits, pandemic

The COVID-19 is a highly transmitted disease by close personal contact or the contact with surfaces. Thus, prevention strategies have been encouraged such as the use of facial masks and adequate hygienization of the hands. In this context, the objective of this study was to evaluate the impact of the hygiene habits changes and the skin care during the pandemic. A literature review was carried out and it was found that while the pandemic have reflected on an increase of hand hygiene, the use of alcohol gel and soap in excess have had negative impacts on the skin due to the damages in the epidermis hydrolipid barrier, which can result in dermatitis and dermatosis. In addition, the use of facial masks has contributed to the skin friction, which can provoke skin face irritation. Therefore, the pandemic had negative impacts on the hydration and integrity of the hand and face skin.

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