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LVI SAIB Meeting - XV SAMIGE Meeting



SAIB-SAMIGE Joint Meeting 2020 – Online

Cover image:

Mineral–microorganisms interactions Mlewski EC¹, Gérard E²

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A Confocal Laser Scanning Microscopy image of a resin-embedded microbialite from Laguna Negra (Puna-Catamarca), stained with calcein (a fluorescent dye that produces a stable complex in the presence of calcium and fluoresces in the green region of visible light). Mineral aggregates are observed in blue. Their surfaces are partially stained with calcein, indicate the presence of free Ca²⁺ ions. Diatoms and *Rivularia halophila* filaments are visible in red thanks to their photosynthetic pigments.

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captured the interest of many researchers trying to develop new medicines. Antiviral bioactivities have been described in numerous medicinal plants and associated with compounds like flavonoids, heterosides, terpenes and triterpenes, organic acids, alkaloids, saponins, and quaternary ammonium salts, among others. The aim of this work was to evaluate compounds of natural origin, mainly from medicinal plants, as potential SARS-CoV-2 inhibitors through docking studies. Molecular docking was performed using AutoDock, with the Lamarckian Genetic Algorithm, to analyse the probability of docking. The viral spike (S) glycoprotein and the main protease Mpro, involved in the recognition of virus by host cells and in viral replication, respectively, were the main molecular targets in this study. These proteins are essential to the transmission and virulence of the virus. By inhibiting anyone of these proteins or both, for a higher active therapy, the severity of the infection will be reduced. Our efforts have been placed in competitively inhibiting the binding of its natural substrates. The best energy binding values for S protein were, in kcal/mol: -19.22 for glycyrrhizin, -17.84 for gitoxin, -12.05 for dicumarol, -10.75 for diosgenin, and -8.12 for delphinidin. For Mpro were, in kcal/mol: -9.36 for spirostan, -8.75 for N-(3-acetylglycyrrhetinoyl)-2-aminopropanol, -8.41 for α -amyrin, -8.35 for oleanane, -8.11 for taraxasterol, and -8.03 for glycyrrhetinic acid. In addition, the synthetic drugs umifenovir, chloroquine, and hydroxychloroquine were used as controls for S protein, while atazanavir and nelfinavir were used for Mpro. Key hydrogen bonds and hydrophobic interactions between natural compounds and the respective viral proteins were identified, allowing us to explain the great affinity obtained in those compounds with the lowest binding energies. These results suggest that these natural compounds could potentially be useful as drugs to be experimentally evaluated against COVID-19. Furthermore, the present study provides molecular details that allow us to propose structural modifications of some compounds to make the interaction between them and viral proteins even more effective.

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CELL WALL MODIFICATION OF THE GREEN ALGA Scenedesmus sp.

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Scenedesmus is one of the most common freshwater algae genera. It can exist as unicellular organism; however, it is also found in *coenobia* organization which consists of four or eight cells inside a parental mother wall. The structure of the cell wall is important because it not only shapes the cell, but it is also the structure that is in contact with the external environment. In particular, *Scenedesmus* has a three-layered cell wall with cellulose, algaenan and pectin. In this work we generated transgenic algae overexpressing carbohydrate binding modules in the cell wall. The transgenic lines obtained are larger than wild type, their surface-to-volume ratio is affected, and the large mass promotes sinking. Cell wall components are altered, specifically the pectin layer, which increases the union between cells forming a conglomerate. We observed a greater laxity of the cell wall and an increase in the amount of pectin, fact that agree with the phenotype of transgenic plants that overexpressed starch binding domains of *Arabidopsis thaliana* starch synthase III. Apart from lack of an efficient harvesting technology, one of the major difficulties in using algae is their recalcitrant cell wall, which, on the other hand, is considered as an excellent food supplement. The presence of sugars in the cell wall following hydrolysis facilitates bioethanol production. Our results suggest that transgenic *Scenedesmus* have an advantage for the production of biofuels in terms of better access to the inner cellulose layer and facilitate its degradation and saccharification.

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SEMI-COMMERCIAL SCALE TEST OF PACKAGING PEARS WITH Vishniacozyma victoriae, YEAST SELECTED AS A BIOLOGICAL CONTROL AGENT

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Pears, as a perishable product, require cold storage for long-term preservation to regulate supply. However, throughout this conservation the fruit is susceptible to different fungal diseases, caused mainly by Botrytis cinerea and Penicillium expansum, therefore, Biological Control is an alternative for the substitution of fungicides, with advantages for environmental sustainability and organic fruit production. V. victoriae was selected in a previous work because of its biocontrol effectiveness against postharvest pears diseases in commercial scale and in situ assays, protected under patent INPI No.: 20120101053. In this work, the yeast biomass was produced from different culture medium, using cheese-whey powder (CWP), cider residue (CR), salts and vitamins, with the intention of replacing expensive inputs. Fermentations were carried out in batch reactor (12 L), the CFU/mL and quality of the yeast biomass were evaluated. The V. victoriae biomass was evaluated through semicommercial-scale assays in a packaging line of pears, spraying 10⁸ cells/mL over 1400 pears. For this, the incidence and disease control percentages caused by phytopathogenic fungi are determined. The biomass both fresh and lyophilized was evaluated and control percentages of fresh and dehydrated biomass grown in SQP were compared. On the other hand, the fresh biomass grown in SQP and RS was compared. Treatments were conserved postharvest in cold rooms (-1/0°C and 95% RH) for 5 months. These tests will establish an ideal condition for the development of fresh and dehydrated biomass. Packham's Triump was the variety tested on a semi-commercial scale. After 120 days, the fresh yeasts grown in CWP provided a control percentage of 58% for the disease caused by P. expansum and 47% for the disease caused by B. cinerea, while the freeze-dried yeasts achieved 65% control at P. expansum and 15% at B. cinerea. On the other hand, the yeasts grown in CR, obtained a