RESEARCHER INFORMATION

Rodrigo Ligabue-Braun
Adjunct professor
Pharmacosciences Department
Universidade Federal de Ciências da Saúde de Porto Alegre (UFCSPA)
Rua Sarmento Leite, 245
Prédio 1, Sala 304C
Porto Alegre, Rio Grande do Sul, Brasil
CEP 90050-170
rodrigolb@ufcpsa.edu.br

PROJECT TITLE: Rocio Virus – Drug modeling and repurposing strategies for a neglected emerging disease

KEYWORDS – *Rocio virus; drug repurposing; drug repositioning; virtual screening*

INTRODUCTION - It is estimated that 15% of all human pathogens are responsible for causing emerging diseases, with 75% of these emerging diseases having a zoonotic origin. These diseases are transmitted from animals to humans by direct contact, water, food, and are most commonly spread by vectors. Among them, we can mention the encephalitis caused by the Rocio virus, an endemic arbovirus belonging to the family Flaviviridae, transmitted by mosquitoes of the species *Psorophora ferox* and *Aedes scapularis*. This encephalitis epidemic in southeastern Brazil lasted from 1973 to 1980, with approximately one thousand cases of the disease, causing about one hundred deaths and two hundred patients with sequelae. Related symptoms include headache, fever, respiratory complications, malaise, and neurological symptoms related to encephalitides, such as blindness, confusion, seizures, deafness, dysarthria, meningitis, and motor and reflex abnormalities. Although the outbreak was limited to the Vale do Ribeira region, in the state of São Paulo, data suggest the circulation of the virus throughout the Brazilian territory, which, together with other sociodemographics and environmental factors, is the circulation of the virus throughout the Brazilian territory, may enable a re-emergence of this disease.

OBJECTIVES – Perform a virtual analysis for the repositioning of drugs to fight infections related to the Rocio virus, in order to: (a) elucidate the structural and non-structural proteins of Rocio virus; (b) determine the possible molecular target(s) and analyze the interaction of drugs already available in the databases integrating the market and the Brazilian Sistema Único de Saúde; (c) identify possible candidates for the treatment of this arbovirosis.

METHODOLOGY – The analysis will be carried out in three stages:

(1) Obtaining the genomic sequence of the NCBI Viral Genomes Resource, under access code NC_040776.1. to elucidate three-dimensional structures for all viral proteins.

(2) Structural protein modeling using mixed techniques, applying classical comparative molecular modeling, together with folding recognition and mold-free approaches. The construction and refinement of the molds will be carried out using the I-TASSER and SwissModel platform platforms.

(3) Selection of potential targets and virtual drug screening based on the literature available for taxonomically close viruses and the degree of identity of viral proteins to human proteins. The analysis will be performed using the database of molecular structures Zinc, and the molecular docking platform DockThor. All drug-target interactions will be inspected via PLIP.

PERSPECTIVES – We hope that this study will allow the identification of possible molecular targets of the Rocio virus and drugs that can be repositioned for the treatment of this neglected emerging disease in a safe and applicable way to the Sistema Único de Saúde based on the elucidation of viral structures.

SIGNATURE