08208 - Poster Session

KA.28 - In Silico Analysis of the A4V and D90A Variants of Human SOD1 related to Amyotrophic Lateral Sclerosis

Gabriel Rodrigues Coutinho Pereira [1], Joelma Freire De Mesquita[1]
[1]Bioinformatics and Computational Biology Group, Federal University of the State of Rio de Janeiro (Rio de Janeiro, Brazil)

INTRODUCTION
Amyotrophic lateral sclerosis (ALS) is the most frequent motor neurodegenerative disorder in adults. Missense mutations in superoxide dismutase 1 (SOD1), a major cytoplasmic antioxidant enzyme, are associated with the development of ALS. The A4V and D90A variants account for approximately half of all ALS-SOD1 cases in the United States and Europe.
OBJECTIVES
This work aims to characterize in silico the structural and functional effects of A4V and D90A variants on human SOD1 protein.
MATERIALS AND METHODS
Three-dimensional structures of A4V and D90A protein variants were computationally modeled in the VMD-1.9.1 package using the experimentally determined structure of wild-type SOD1 (PDB ID: 2C9V) as the template. Molecular dynamics (MD) simulations of the wild-type SOD1 protein and its variants A4V and D90A were performed in triplicates using the GROMACS-2018.8 package and AMBER99SB-ILDN force-field. TIP3P water molecules were added to a dodecahedral box system, which was neutralized by the addition of Na+ Cl- ions and then minimized. The system also had its temperature and pressure equilibrated at 1atm and 300K before the start of the simulations, which lasted 300ns. The MD trajectories were concatenated, and the following parameters were analyzed using GROMACS distribution programs: root-mean-square deviation, root-mean-square fluctuation, B-factor, radius of gyration, solvent accessible surface area, secondary structure, and essential dynamics.
DISCUSSION AND RESULTS
The MD analyses pointed to changes in flexibility and essential dynamics in the regions corresponding to the electrostatic and metal-binding loops of the variants, which could impact substrate guidance towards the active site and their enzymatic activity.
CONCLUSION
Our findings pointed to structural alterations in A4V and D90A variants that could have functional implications for SOD1 and explain their association with the development of ALS.
Keywords: Amyotrophic Lateral Sclerosis, Superoxide Dismutase 1, In Silico
Supported by: FAPERJ, CAPES, DAAD, FINEP, NVIDIA, CNPq and UNIRIO

08779 - Poster Session

KA.29 - Evaluation of chemical elements distribution and their inter-elemental correlations in tumor progression

Samella Pontes Salles[1], Simone Coutinho Cardoso[2], Mauro Sérgio Gonçalves Pavão[2], Mariana Paranhos Stelling[1]
[1]Núcleo de Ciências Biomédicas Aplicadas, Instituto Federal de Educação, Ciência e Tecnologia do Rio de Janeiro (, Brazil), [2]Instituto de Bioquímica Médica Leopoldo De Meis, Universidade Federal do Rio de Janeiro (, Brazil)

INTRODUCTION
Cancer is considered one of the most complex and fatal diseases worldwide. New approaches to study tumor progression and growth are relevant subjects of research. In this context, the particular role of chemical elements in cancer progression is a subject still not fully explored that presents opportunities for investigation.
OBJECTIVES
The main goal of our study is to assess the distribution of chemical elements in cancer progression as well as to discover correlations between elements, observing both the primary tumor and the distant tissues that the tumor cells may affect.
MATERIALS AND METHODS
For simulating tumor progression in vivo, murine Lewis lung carcinoma cells were injected in C57BL/6 mice and data indicating the presence, concentration, and location of different elements in distinct tissues, in both control and experimental groups, were obtained in a time frame of 5 weeks of tumor progression. The data were collected via Synchrotron Radiation X-Ray Fluorescence in the Brazilian Synchrotron Light Laboratory (LNLS). In order to extract relevant information inherent to the voluminous available data, we adopt statistical analysis.
DISCUSSION AND RESULTS
With this work, it was possible to observe the elements' relevance for biological processes of normal, as well as tumor cells, during its tumor progression. Thus, it was possible to notice indications of tumor influence on distant tissues as well as highlight the importance of elements and their correlations for the tissues, including for processes of tumor progression, such as growth and cellular migration, angiogenesis, among others.
CONCLUSION
This work also confirmed information found in the literature and featured results apparently not yet observed. Moreover, elements and correlations of relevance for more investigation, regarding their role in the processes described, were highlighted to bring to light explanations for such observations not yet noted.
Keywords: elemental distribution, tumor progression, X-Ray fluorescence

08524 - Poster Session

KA.30 - POLYana: a new software for rheological study of polymeric colloidal materials

Anderson Ferreira Sepulveda [1], Margareth Franco[2], Fabiano Yokaichiya[3], Daniele de Araujo[1]
[1]Center for Natural and Human Sciences, Federal University of ABC (São Paulo, Brasil), [2]RMB, Nuclear and Energy Research Institute (São Paulo, Brazil), [3]Physics Department, Federal University of Parana (Parana, Brazil)

INTRODUCTION
POLYAna is a new executable software developed by SISLIBIO group for rheological analysis of hydrogel and organogel systems and other colloidal materials (nanoparticles and micelles). The software development aims to facilitate the analysis of rheology data associated to both temperature- and frequency-dependent analysis, viscosity and curve flow profiles.
OBJECTIVES
The software development aims to facilitate the analysis of rheology data associated to both temperature- and frequency-dependent analysis, viscosity and curve flow profiles.
MATERIALS AND METHODS
From raw data, several models are applied like power-law model for frequency response and curve flow, Boltzmann law to calculate gelation temperature and viscosity response under temperature, Maxwell model to study interchain relationships in addition to other models such as Bingham model, Cross model, and Herschel-Bulkley are also available. POLYana outputs calculates rheological parameters like consistency, adhesion, hysteresis, flow index, G'/G" ratio.
DISCUSSION AND RESULTS
To validate results obtained from POLYana, same data were analyzed by applying other programs and same mathematical models. In this sense,

rheological analysis of Poloxamer 407 in water solution (15 %) were performed: from temperature-dependent G' and G" analysis were obtained gelation temperature of 45.46 ± 0.02 °C, η_0 = 0.08 ± 0.03 mPa*s, η_max = (32.44 ± 0.17) mPa*s and dη/dT = (1.27 ± 0.02) mPa*s/°C by fitting Boltzmann law (R2 = 0.998), which are similar to results obtained by others softwares and found in literature. From temperature-dependent G' and G" analysis, it gets adhesion value of (1647.15 ± 18.01) mPa*sn calculated from power-law model (R2 = 0.869), also similar to PRISM results.
CONCLUSION
Also, other Poloxamer concentrations and hydrogels types have been evaluated, showing close numbers to that previously reported. In order to stablish structural relationships, one of POLYana tools is also to analyze small-angle neutron scattering (SANS) and develop Monte Carlo simulation for SANS and rheological analysis, simultaneously.
Keywords: Colloidal materials , Rheology, Software
Supported by: CAPES (grant #001), CNPq (307718/2019-0)

08871 - Poster Session

KA.31 - Strategies of Ranking methods for Virtual Screening in SARS-CoV-2 PLpro
Bruce Veiga Andriolo [1,2], Caio Felipe de Araujo Ribas Cheohen[1,2], Diego Henrique Silvestre[1], Manuela Leal da Silva[1,2]
[1]Instituto Nupem, Universidade Federal do Rio de Janeiro (Rio de Janeiro , Brazil), [2]Diretoria de Metrologia Aplicada as Ciências da Vida, Instituto Nacional de Metrologia, Qualidade e Tecnologia (Rio de Janeiro , Brazil)

INTRODUCTION
In 2019 strange cases of unidentified pneumonia led to the discovery of a new species of coronavirus, the SARS-CoV-2 responsible for COVID-19 pandemic. One of its most important proteins is the PLpro for its ubiquitin and deISGylating capabilities. Considering the costs of developing new drugs, repositioning already approved drugs is an excellent strategy in fighting COVID-19. We used the drugs approved by the Brazilian Health Regulatory Agency ANVISA using *in silico* techniques to try to predict interaction between these compounds and the PLpro. The importance of this work is based on the huge amount of money and time needed to develop a novel drug, while repositioning is cheaper and faster.
OBJECTIVES
Perform Virtual Screening and use different strategies for ranking the results to determine possible candidates to inhibit SARS-CoV-2 PLpro.
MATERIALS AND METHODS
Virtual Screening was performed by AutoDock Vina using parameters defined in redock with the exception of generation of 20 poses. After VS the candidates whose energy was lower than -8.0 kcal/mol were selected. For ADMETox prediction, SwissADME, admeSAR and pkCSM were used with PAINS and AMES being considered as limiting factors. The distance between the molecules and Y268 from PLpro was measured using PyMOL and molecular weight was used like a filter. The compounds were ranked based on these criteria.
DISCUSSION AND RESULTS
From the original 273 compounds, 44 had the correct energy range. From those, 36 passed the AMES and PAINS test who were ranked and organized in accordance with their usage. Vitamins, unpromising or problematic drugs were excluded.
CONCLUSION
Using ADMETox prediction and information about distance, pocket volume and literature we organize possible drugs to be tested *in vitro* against PLpro of SARS-CoV-2 and HEK-293 lineage cells.
Keywords: SARS-CoV-2, PLpro, Virtual Screening
Supported by: CNPq and CAPES

08572 -

KA.32 - Immunogenic characterization of the antigen group (gag) gene of strains of the human immunodeficiency virus type 1 (HIV-1) circulating in Brazil,
STEVE BIKO MENEZES HORA ALVES RIBEIRO [1]
[1]Biofunção, Universidade Federal da Bahia (BA, Brasil)

INTRODUCTION
A large genetic variability of HIV represents a major obstacle to the control of infection by the host immune system and to the development of effective drugs and vaccines. CTLs recognizing epitopes within the HIV antigen (gag) group gene have been associated with the initial control of infection and these epitopes, uses in current approaches to developing an HIV vaccine.
OBJECTIVES
This study aims to investigate a variability of the non-gag HLA class I ligand binding epitopes of circulating HIV-1 strains in Brazil, available in a publicly accessible database.
MATERIALS AND METHODS
For this purpose, an allelic variability and predominance of HLA class I in the Brazilian population was determined in order to identify the epitopes of the gag gene of circulating HIV-1 strains in Brazil. One was evaluated by target cell (CTL / CD8) and one screened by an assessed target cell (CTL /CD8). , the already defined gene (gag) and the most prevalent HLA alleles in the Brazilian population. The Allele Frequency Net Database (AFND) was used, as gag regions were removed from through the electronic address https://www.hiv.lanl.gov, with the defined genes (gag) and the alleles most prevalent in the Brazilian population. The Immune Epitope Database (IEDB) was used to determine which are the best Brazilian HLA-linked epitopes.
DISCUSSION AND RESULTS
From this research a table with a description of the non-Brazilian circulating epitopes was generated for each HLA class I allele to the HIV-1 subtype and position of the epitope in relation to the gag gene.
CONCLUSION
Thus, it is concluded that the variability of HLA class I ligand epitopes in the gag gene found, generated a sum of importance data to characterize and describe the non-circulating epitopes in Brazil and to show the studies involved with these epitopes not the world, for future future vaccine referrals in Brazilian territory.
Keywords: HIV, Epitopes, Brazil

08518 - Poster Session

NB.01 - Synthesis of a iodine-131-labeled derivative of laminin-111, [131I]I-YIKVAV, and its assessment as a potential radiopharmaceutical for breast cancer diagnosis
Fernanda Ferreira Mendonça [1], Danielle Vieira Sobral[1], Ana Claudia Ranucci Durante[2], Ana Claudia Camargo Miranda[2], Jorge Mejia[2], Wagner Ricardo Montor[1], Marycel Figols de Barboza[2], Leonardo Lima Fuscaldi[1], Luciana Malavolta[1]
[1]Departamento de Ciências Fisiológicas, Faculdade de Ciências Médicas da Santa Casa de São Paulo (Sao Paulo, Brasil), [2]Instituto Israelita de Ensino e Pesquisa, Hospital Israelita Albert Einstein (Sao Paulo, Brasil)

INTRODUCTION
Peptide sequences derived from laminin-111 regulate gene expression in breast tumor cells, including the bioactive peptide IKVAV.
OBJECTIVES
Here, we evaluated the potential of the YIKVAV modified fragment radiolabeled with iodine-131 by *in vitro* interaction with human breast cancer cells and *ex vivo* biodistribution in mice.