Conesul Symposium on Biomolecular Simulations - CSBS
VIII Congresso Regional da SBBf

	31/05	01/06	02/06
09:00hs		**Dario Estrin** QM-MM simulations using the ANI machine learning potential: assessment of embedding schemes	**Ariela Vergara** Understanding the impact of protein-protein interactions on TRP ion channel function: A computational approach
09:30hs	Registration / Openning		
10:00hs	**Paulo Bisch** From picosecond to millisecond (or more): 40 years of (bio-) molecular dynamics simulations	**Munir Skaf** Collision Cross Section Calculations of Biomolecular Assemblies in Ion Mobility Mass Spectrometry	**Viviana Monje** Protein-lipid fingerprints: realistic membrane modeling using atomistic simulations
11:00hs	**Adrian Roitberg** Machine Learning in Chemistry. Are the Robots coming for our jobs?	Coffee-Break	Coffee-Break
11:30hs		**Margot Paulino** From AI to Medicinal Chemistry: the design of novel anti trypanosomatids	**Flavio Seixas** Identification of inhibitors for SARS-CoV-2 main protease from plant extracts. In silico and in vitro studies
12:30hs	Lunch	Lunch	Lunch
14:00hs	**Lucianna Santos** Coarse-grained simulations of a virus like particle with the SIRAH force field	**José F. Bachega** Exploring enzymatic reactions using EasyHybrid	**Jose Colbes** Recent advances in protein structure prediction and peptide design
15:00hs	Poster section	Poster section	Apresentação oral trabalhos selecionados
16:00hs	Coffee-Break	Coffee-Break	Coffee-Break
16:30hs	Poster section	Poster section	Oral presentation of selected students
18:00hs			Closing section