**Mauricio Menegatti Rigo**

*Developing Structural Tools for Immunotherapy Improvement*

Immunotherapy treatments have revolutionized the clinical approach for patients with cancer. Contrary to conventional approaches such as chemotherapy, immunotherapy is designed to improve the competence of immune cells against cancer cells. In this scenario, T-cell lymphocytes are able to recognize tumor-derived peptides displayed at the surface of cancer cells by Human Leukocyte Antigens (HLAs), promoting the tumor elimination. Although there exist computational pipelines designed to identify and suggest new tumor-specific peptide-targets that activate specific T-cell lymphocytes receptors (TCRs), undesired outcomes such as low affinity T-cells and immune evasion hamper progress in this field. We hypothesize this happens mainly because computational methods do not take into account the protein flexibility between the peptide-HLA complex (pHLA) and the TCR. Our goal is to create a platform that allows practitioners with different expertise to perform protein-protein molecular docking using ensembles of pre-computed conformations from pHLAs and TCRs.