# HOW CAN BIOINFORMATICS TOOLS HELP TARGET NEW IMMUNOGENS? AN *IN SILICO* ANALYSIS OF TWO KNOWN IMMUNOGENIC CHIMERA PROTEINS FROM *ASCARIS* SP.

TATYANE MARTINS CIRILO[1], JOSÉ BRYAN DA ROCHA RIHS[1], ANA CRISTINA LOIOLA RUAS[2], LILIAN LACERDA BUENO[1,2], JONI ESROM LIMA[3], RICARDO TOSHIO FUJIWARA[1,2]

[1]POSTGRADUATE PROGRAM IN PARASITOLOGY, FEDERAL UNIVERSITY OF MINAS GERAIS, MINAS GERAIS, BRAZIL, [2]POSTGRADUATE PROGRAM IN TROPICAL MEDICINE, FEDERAL UNIVERSITY OF MINAS GERAIS, MINAS GERAIS, BRAZIL, [3]POSTGRADUATE PROGRAM IN BOTANY, FEDERAL UNIVERSITY OF MINAS GERAIS, MINAS GERAIS, BRAZIL

Ascariasis, a neglected disease caused by parasites of the genus *Ascaris*, affects millions of people and has high morbidity rates. Due to the recurrence of reinfections, even after drugs treatment, a vaccine is essential for the control of the disease. This study aims to evaluate the immunogenic potential of two *Ascaris* proteins previously studied as vaccine candidates. Using bioinformatics tools, the proteins were evaluated for their physicochemical properties, ability to induce immune response and immunogenic potential. The physicochemical properties were analyzed by ProtParam and Protein-Sol, the immunogenicity was predicted by VaxiJen and the immune response was simulated by C-IMMSIM. Tertiary structure prediction was carried out using I-TASSER. The BOT sequence (217 amino acids, 22 kDa) showed a pI of 4.48, stability (instability index: 35.92) and solubility (predicted solubility: 0.924). Immunogenicity was classified as high (1.0778), with simulation indicating an increase in IFN-γ, active memory Th cells and memory B cells. The tertiary structure showed low similarity (C-score of -4), with a predominance of α-helix regions. The ASC-VAC sequence (382 amino acids, 39 kDa) had a pI of 10.04, high instability (74.30) and solubility (0.719). It was classified as immunogenic (0.5057), with a robust simulated response, an increase in IFN-γ, TGF-β, memory Th cells and persistent B cells. The tertiary structure prediction obtained a C-score of -0.30 and a Tm-score of 0.67±0.12, with several α-helix, β-sheet and active site regions characteristic of proteins rich in molecular recognition domains. *In silico* analyses confirm the physicochemical properties and immunogenicity of the proteins, reinforcing the viability of the sequences as vaccine candidates, with the potential to induce a long-lasting immune response. The C-IMMSIM simulations indicate the best time for cellular evaluation, allowing further analysis to ensure the safety and efficacy of the immunogens.

Supported by: CAPES, CNPq

Keywords: Ascariasis. Vaccine. Computacional Biology.