Contribution ID: **35** Type: **Poster (sponsored)**

Identification of potential Bruton's tyrosine kinase inhibitors for the treatment of rheumatoid arthritis using computational drug discovery methods

Rheumatoid arthritis (RA) is a chronic systemic autoimmune disease of the synovial membranes affecting multiple joints and often results in extra-articular manifestations. It is characterised by joint deformation and destruction of the cartilage, ligaments and tendons. A cross-sectional meta-analysis study revealed that RA was most prevalent in the South African urban population compared to other African countries. Resistance to disease modifying antirheumatic drugs and biologics necessitates the need for new drugs to treat RA. Bruton's tyrosine kinase is involved in the signalling pathway of osteoclasts, B cells and T cells which are involved in the perturbation of rheumatoid arthritis and makes it an ideal drug target. The study aims to identify potential Bruton's tyrosine kinase inhibitors for the treatment of RA using pharmacoinformatics approaches including pharmacophore-based virtual screening, molecular docking and molecular dynamics. For this purpose, a set of 103 Bruton's tyrosine kinase inhibitors were collected from the Binding database and a number of pharmacophore models developed. The well-validated models were used to screen the small molecule databases. Initially more than a thousand hits were retrieved. A number of criteria including molecular docking and pharmacokinetics will be used to identify the best promising molecules for therapeutic application in RA. The final selected molecules will be evaluated further in molecular dynamics studies and binding energy calculations using MM-GBSA.

Presenter Biography

Primary authors: Ms GOROGODO, Nyasha (University of Pretoria); Dr ISLAM, Ataul (University of Pretoria); Prof. PILLAY, Tahir (University of Pretoria)

Presenter: Ms GOROGODO, Nyasha (University of Pretoria)

Session Classification: Poster session

Track Classification: Bioinformatics and Biological Sciences