In silico study on mansonone G analogs against Janus kinase 2 for developing anticancer agents
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Abstract: The Janus kinase 2 (JAK2) provides an instruction for making a protein that promotes the growth and division (proliferation) of cells. This protein is involved with signal transduction pathway, called the JAK/STAT pathway, which transmits chemical signals from outside the cell into the cell. The JAK2 protein is especially important for controlling the production of blood cells from hematopoietic stem cells. The myeloproliferative neoplasms (MPNs) comprise of a group of clonal stem cell disorders associated with a high prevalence of mutations in JAK2, overproduction of mature blood elements, and variable rates of transformation to acute myeloid leukemia (AML). In this research, the 20 analogs of mansonone G (MG) were focused for molecular screening towards JAK2 protein. Molecular docking study was performed by the CDOCKER (Discovery Studio 2.5). The binding affinity of all MGs were ranked and compared with the known inhibitors. The results revealed that MG4 (-53.06 kcal/mol) and MG14 (-52.97 kcal/mol) showed stronger binding affinity against the JAK2 than ruxolitinib (-41.69 kcal/mol). The obtained data suggested that these two compounds might be used as a template for developing anti-cancer agents against JAK2.

Keywords: JAK2; Mansonones; Molecular docking