In Silico Study of Andrographolide, a Diterpenoid Compound from Herba Sambiloto (*Andrographis paniculata*(Burm.F) Nees), with NF-*kappa*B Molecule

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ABSTRACT

Molecular docking represents molecular modeling techniques which are used to predict how any macromolecules (typically a protein) interact with other molecules (may be other proteins, nucleic acids or small drug-like molecules). The purpose of this study is to visualize the interaction of andrographolide, a major active compound of Andrographis paniculata (Burm.F) Nees, and its molecule target, NF-kappa B, at molecular level, and predict its inhibition constant, to understand its antiinflammatory activity. The softwares used in this study are ChemOffice 2008, OpenBabel, SwissPDB Viewer and AutoDock Tools 3.05 that consists of AutoGrid and AutoDock. Docking was applied to p50 and p65 subunits of NF-kappaB. Based on Lamarckian Genetic Algorithm used in this study showed that p50 subunit of NF-kappaB is a possible binding site for andrographolide. The present findings may represent an important advance for understanding the antiinflammatory mechanism of andrographolide.

Keywords : *docking, andrographolide*, NF-*kappa*B, *AutoDock*

ISBN No. 978-979-25-1207-6