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# Molecular interaction studies of Anthraquinone derivatives, potent anticancer agents from the root of *Morinda citrifolia* (Noni)

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In the era of stressful life, different food habits associated with drug resistance, has lead to search for alternative health drinks. *Morinda citrifolia*, a plant from Rubiaceae family is available as a health tonic, also known as Noni juice in India. This juice has natural resources like Anthraquinone compounds extracted from root of *Morinda citrifolia*. This has reported anticancer properties through in vitro studies for antitumorigenic activity. Their potential target is $p56^{lck}$, a protein essential for the development of T-cells and activity involved in the chemotactic responses of these cells. This protein is reported to play crucial role in breast cancer and colon cancer. Anthraquinones acts as a potent inhibitors of $p56^{lck}$ tyrosine kinase receptor in human cancer cells. Among anthraquinones derivatives, Damnacanthal was proved to induce cell growth arrest and trigger caspase activity in colorectal cancer cells and it is a potent inhibitor of $p56^{lck}$ tyrosine kinase activity. Till date, molecular level interactions between the anthraquinones and the receptor protein were not reported from *in silico* perspective. In the present study, we investigated the molecular interactions between Anthraquinones from the root of Noni with $p56^{lck}$ receptor using AutoDock's Lamarckian genetic algorithm. Here we studied the binding site and behavior of 20 anthraquinones including Damnacanthal within the catalytic domain of $p56^{lck}$ receptor. Our results reports that apart from Damnacanthal, all other anthraquinones exhibits similar interactions in the active site of $p56^{lck}$ receptor and we proposed the molecular models of these anthraquinones with the receptor. Thus to conclude, the compounds derived from the root of Noni plant showed promising molecular specificity and interactions with the receptor involved in cancer cells.

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