

## Anticancer Lantadene Derivatives: Synthesis, Cytotoxic and Docking Studies

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**Abstract :** Nuclear factor-kappa B serve as a molecular lynchpin that links persistent infections and chronic inflammation to increased cancer risk. Inflammation has been recognized as a hallmark and cause of cancer. Natural products present a privileged source of inspiration for chemical probe and drug design. Herbal remedies were the first medicines used by humans due to the many pharmacologically active secondary metabolites produced by plants. Some of the metabolites like Lantadene (pentacyclic triterpenoids) from the weed *Lantana camara* has been known to inhibit cell division and showed anti-antitumor potential. The C-3 aromatic esters of lantadenes were synthesized, characterized and evaluated for cytotoxicity and inhibitory potential against Tumor necrosis factor alpha-induced activation of Nuclear factor-kappa B in lung cancer cell line A549. The 3-methoxybenzoyloxy substituted lead analogue inhibited kinase activity of the inhibitor of nuclear factor-kappa B kinase in a single-digit micromolar concentration. At the same time, the lead compound showed promising cytotoxicity against A549 lung cancer cells with IC<sub>50</sub> ( half maximal inhibitory concentration) of 0.981  $\mu$ M. Further, molecular docking of 3-methoxybenzoyloxy substituted analogue against Inhibitor of nuclear factor-kappa B kinase (Protein data bank ID: 3QA8) showed hydrogen bonding interaction involving oxygen atom of 3-methoxybenzoyloxy with the Arginine-31 and Glutamine-110. Encouraging results indicate the Lantadene's potential to be developed as anticancer agents.

**Keywords :** anticancer, lantadenes, pentacyclic triterpenoids, weed

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