Synthesis, Biological Evaluation and Docking studies of Substituted 4-Thiazolidinone Derivatives as Antioxidant, Anti-inflammatory and Anticancer agents

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Abstract

In drug discovery and development heterocyclic scaffolds play a major role. Nowadays, various heterocyclic scaffolds, like thiazole, thiazolidinones, or thiazolidinedione have been successfully proven to be effective against cancer and inflammation. The present research reports synthesis of ten 4-thiazolidinone derivatives via three step synthesis. The structural confirmation of the compound was found through Spectrophotometric analysis such as Mass spectrometry, NMR, IR spectroscopy. Also, the synthesized compounds were found to possess anti-oxidant, anti-inflammatory and anti-cancer properties. All the synthesized compounds have good to moderate antioxidant activity with maximum rummage being possessed by P7 and P10. The carrageenan-rat paw edema method was used to determine *in-vivo* anti-inflammatory activities and the compounds P4 and P7 showed maximum inhibition. The synthesized derivatives showed *in-vitro* anti-tumor activity against MOLT-4, EAC cell lines, the results showed that the compounds P4, P7 and P10 came out as the most remarkable analog against the above-mentioned cell lines. The molecular docking studies by using auto-dock 4.2.6 software and SAR (structure-activity relationships) has shown that title compounds such as electron donating groups (OH or OCH_3) groups arylidene ring at position-5 enhances the anti-oxidant activity whereas the electron withdrawing group diminishes the same. Chloro substituted phenyl amino group present at the second position increases the anti-inflammatory activity whereas attaching electron donating group on arylidene moiety at 5^{th} position of 4-thiozolidione enhanced the anti-cancer activity.