



**Original Research Paper**

## **Quantum Chemical Study of Interaction of PLGA Polymeric Nanoparticles as Drug Delivery with Anti-Cancer Agents of Thiazoline**

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### **ABSTRACT**

Thiazoles derivatives are consisted in chemical compounds such as antimicrobial and anticancer medicine. Since polylactic-co-glycolic acid (PLGA) polymeric nanoparticles has been conversed about nanomedicine applications and particularly as drug delivery systems. Because of molecular self-assemblies and biodegradability of PLGA polymer, it can be used to carry anti-cancer and antimicrobial drugs. The capability of PLGA polymer-based drug delivery system in the treatment of cancer has been studied by quantum MM/QM approach. Theoretical study of the interaction between polylactic-co-glycolic acid polymeric nanoparticles and thiazoline derivatives has been performed by combination of DFT and molecular mechanics approach. The results obtained from this study, displayed that PLGA polymeric nanoparticles has feasible interaction that include hydrogen bond and Vander Waals interaction and showed clearly that these systems have comparatively low permanence and so PLGA polymer is suitable drug delivery that have been studied for anti-cancer drug. Investigation of QM/MM calculations and the interaction energies of the thiazoline derivatives and PLGA polymeric nanoparticles with