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Ab Initio study on nano carrier (*RS*)-2-(1,2,3,4-tetrahydronaphthalen -1-yl)-4,5-dihydro-1*H*-imidazol drug about Substituted effect in energy levels, dipole moment and structural parameters

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Abstract

Tetryzoline(TH) is an adrenergic agent (vasoconstrictors) and derived from imidazoline. This compound is closely related to naphazoline hydrochloride in its pharmacological action. Nanotechnology has been used to provide advanced biomedical research tools in drug delivery. The fullerene family especially C60 derivatives have appealing photo-, electro-chemical and physical properties for biomedical applications. In this report, at the first Tetryzoline drug located on fullerene and halogen derivatives (in carbon position 69) [C60- Tetryzoline – C69-X] (X=F, Cl, Br) were optimized. Then the calculation of natural bond orbital was performed with the NBO technique. All calculations using Hartree- Fock the 6-31G * basis set using Gaussian 98 software and in gas phase has been done. The results showed that the energy levels of molecular orbitals (HOMO & LUMO) in the R-F have the lowest value. C69-F is shortest bond and most Strength. Comparison of the dipole moment of compounds shows this trend: R-F> R-Cl> R-Br.

Keywords: Tetryzoline , nano carrier, fullerene , dipole moments.

1. Introduction