A QUANTUM MECHANISTIC STUDY INTO THE CHEMO AND REGIO-SELECTIVITY IN THE SYNTHESIS OF ISOXAZOLINE AND ISOXAZOLE DERIVATIVES

Isoxazoline compounds have been recognized for their notable biological significance in various studies but have serious side effects such as ataxia, muscle tremor and seizure. Combination of Isoxazoline with chromene derivatives turn to have great biological activities towards many diseases and eliminates these side effects. The synthesis of these scaffolds is only achieved through condensation reaction which renders the products impure due to the formation of byproducts which sometimes further react with the product under the same reaction condition. Use (3 + 2) cycloaddition (32CA) reaction method for the synthesis of these scaffolds using Kumar et al experimental work. The chemo-selectivity between nitrile and olefinic functional groups, and underlining molecular reaction path for the [3 + 2] cycloaddition reactions of phenyl nitrile oxide(dipole) with (E)-2-amino-4-argio-8-(argiomethylene)-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile(dipolariphile) derivatives must been investigated by employing suitable levels of density functional theory.

OBJECTIVES

Study the 32CA reaction of (E)-2-amino-8-benzylidene-4-phenyl-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile with nitrile oxide, to understand the drive towards the chemo- and Regio-selective addition across the ethylene site by running global and local descriptors calculations. Also explore possible reaction channels, and the effect of electron releasing groups (ERG), electron withdrawing groups (EWG), solvents and temperature on the reactions' outcomes, towards gaining control over the product formed at reaction equilibrium.