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A computational study of mechanistic pathways for the design of a greener process in the production of quinoline-2-(1H)-one and its derivatives

Quinolinones are heterocyclic aromatic compounds with various pharmacological activities. Their importance has brought about the need for green synthetic methods [1]. Exploring greener pathways using an experimental trial and error approach is costly and hazardous hence computational investigations of the existing mechanistic pathways are an alternative [2]. This study focused on the computational study of a fast, base-free aqueous synthesis of quinolin-2(1H)-one. Molecular simulations were done using DFT [3], MP2, and CCSD(T) [4] to obtain reaction energy profiles of quinoline-2(1H)-one in gas, water, and dichloromethane with the aid of Gaussian 16 revision C01[5]. The computational simulations were conducted at the Centre for High Performance Computing (CHPC). The jobs were submitted for execution on a single node with 24 cores and a specified memory of 10GB. The scheduled wall times utilized varied between 10-96 hrs for optimisation and normal mode analysis, which were executed as two separate simulations for each species investigated. The profiles for the two-step reaction helped to elucidate the energy barriers for the chemical reaction. The barrier for the reaction in water and dichloromethane in the first step was 22.44 and 20.58 kcal/mol, respectively, while for the second step 27.24 and 28.35 kcal/mol was obtained. HOMO-LUMO analysis and quantum theory of atoms in molecules (QTAIM) calculations were explored to provide further insight into the reaction. The energy gap for the final product was 0.249 eV indicating a relatively stable molecule which could possibly participate in other reactions. The stability was supported by average rho and Laplacian of 0.253 and -0.558, respectively, via QTAIM analysis.

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