1 Abstract

This study employs computational analysis to investigate the properties of a series of arylidene indanone molecules (M1-M10). Through quantum calculations and molecular modeling, we explore the intricate relationship between molecular structure and various chemical characteristics. Electronic properties, including orbital energies, HOMO-LUMO levels, and electron density distribution, offer insights into the molecules' potential for interactions and reactivity. Reactivity assessment and barrier analysis, not only enhances our understanding but also facilitates the design of novel derivatives with improved properties. These findings provide valuable guidance for researchers in drug design, materials science, and organic synthesis. By leveraging computational insights, tailored arylidene indanone derivatives can be developed for specific applications. Overall, this study enriches our understanding, propels molecular design, and anticipates the creation of innovative compounds with enhanced attributes for diverse applications.