

Abstract Submitted
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Stereochemical and Thermodynamic Analysis of Retinoids and Fullerenes Used in the Treatment of Acne EUNA JANG, RICHARD KYUNG, CRG-NJ — Studies on the role oxidative stress plays in the pathogenesis of acne vulgaris have suggested that antioxidants may be useful in the treatment of acne vulgaris. A few nanoparticles such as fullerenes and retinoids, prized for their electron-transport capacities, small size, and antioxidant abilities, have thus been considered to be a potent therapeutic agent. Numerous studies validating nano scaled molecules potential to be used in the treatment of acne vulgaris have led scientists to assess the safety of retinoids and fullerene derivatives. In this study, computational biomedical simulation technology has been used in assessing the thermodynamic stability of such molecules. Computer simulations to model the complexes that can virtually attach large quantities of protons and donate electrons to ROS-affected cells. Thermodynamical and stereochemical safety of several types of water-soluble fullerene derivatives that could be used as biological agents in acne treatment were studied. We used a molecular editing program to model, optimize, and compare the resulting molecular optimization energies and other factors of the molecules.

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