

Abstract Submitted
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Thermodynamic Analysis of Surface Functionalized Fullerenes in Treating Acne Vulgaris SE RI LEE, Choate Rosemary Hall — Acne vulgaris is a common skin disease with a multifactorial pathogenesis, including follicular hyperproliferation, sebaceous hyperplasia, commensal bacteria, and inflammation. Recent research has attributed oxidative stress to be a possible cause of this disease, spurring studies assessing the use of fullerene derivatives as antioxidant agents in treating acne. The purpose of this project is to study the potential use of fullerene derivatives in acne therapy. Hydrophilic functional groups were added to fullerene molecules due to the hydrophobic nature of fullerenes. A computational chemical software measured the optimized geometries and chemical properties of the modeled structures by using theoretical values and considering the molecules atomic properties. The efficiency of these molecules was determined by assessing their thermodynamic stability, and surface functionalization was studied to determine its effects on the modification of the biocompatibility of the material itself. The stereochemistry of PVP-F (Polyvinylpyrrolidone Fullerene) and N-methyl pyrrolidine fullerene (NMP-F) molecules were studied to assess their chemical properties including thermodynamic stability.

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