

Abstract Submitted  
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**Study on the Role of Biochemical Fullerene Derivatives in Treating Tumor Cells** JI HAN YOON, GENE PARK, JOSEPH SHIN, Choice Research Group — Substituted fullerenes tagged with a functionalized group or an antibody such as an organic functional group can target cancer cells. In this paper, we compared the molecular energy of fullerenes doped with clusters such as hydroxyl(OH), carboxyl(COOH), and malonic acid(C-COOH) derivatives. When comparing BB derivatives (BB7, BB8, BB9) on C40 and C72 fullerene models, C72 derivatives were observed to have much lower optimization energy levels (kJ/mol) than derivatives of C40. Although the C72 BB derivatives may have a larger number of carbon atoms than the C40 BB derivatives, the C72 BB derivatives possess a more spherical shape, which yields to lower enthalpy. Thus, within the BB derivatives of C40/C72 fullerenes, the phenomenon of C72 models having overall lower optimization energy can be attributed to the C72 models rather spherical and stable shape. When comparing hydroxyl (OH), carboxyl (COOH), and C-COOH derivatives on C40 fullerene models, carboxyl derivatives were observed to have much lower progressing optimization energy levels (kJ/mol) than those of hydroxyl derivatives, with hydroxyl derivatives having much lower progressing optimization energy levels than those of C-COOH derivatives.

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