

DNA/RNA Fragmentation and Cytolysis in Human Cancer Cells Treated with Diphthamide Nano Particles Derivatives

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Molecular structure activity studies for some Diphthamide Nano particles derivatives indicate that the conformational characteristics along with the nature and position of the substituents on the Diphthamide Nano particles derivatives ring play an important role in their biological and biochemical activities (Figure 1) [1-7]. Therefore, we have calculated the optimized molecular geometries of some Diphthamide Nano particles derivatives. Calculations are carried out on the structures of these medical, medicinal and pharmaceutical Nano drugs using Hartree-Fock calculations and also Density Functional Theory (DFT) by performing HF, PM3, MM2, MM3, AM1, MP2, MP3, MP4, CCSD, CCSD(T), LDA, BVWN, BLYP and B3LYP levels of theory using the standard 31G, 6-31G*, 6-31+G*, 6-31G(3df, 3pd), 6-311G, 6-311G* and 6-311+G* basis sets of the Gaussian 09. The comparative heats of formation and Natural Bond Orbital (NBO) charges are calculated for these Diphthamide Nano particles derivatives. We have finally obtained some conformational rules in terms of the natures and positions of the substituents on the Diphthamide Nano particles derivatives ring.

On the other hand, Diphthamide Nano particles is an interesting medical, medicinal and pharmaceutical Nano drug which has received a lot of interests because of its applications in many areas of medical, medicinal and pharmaceutical chemistry. During the last three decades,

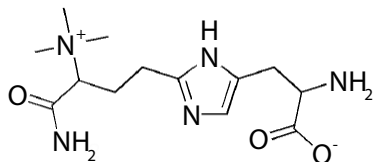


Figure 1: Molecular structure of Diphthamide Nano particles [1-7].

a large number of substituted Diphthamide Nano particles derivatives have been claimed to have several biological and biochemical activities. Molecular structure activity studies for some Diphthamide Nano particles derivatives indicate that the conformational characteristics along with the nature and position of the substituents on the Diphthamide Nano particles derivatives ring play an important role in their biological and biochemical activities. In the course of our studies, we have investigated the chemistry and pharmacology of some Diphthamide Nano particles derivatives. In the present editorial, we have calculated the optimized molecular geometries of some Diphthamide Nano particles derivatives.

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