عنوان مقاله:

Computational study of Anticancer Dasatinib for drug delivery systems

محل انتشار:

کنفرانس ملی نانو ساختارها علوم و مهندسی نانو (سال: 1398)

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خلاصه مقاله:

Dasatinib is a tyrosine kinase inhibitor (TKI) that is used to treat chronic myeloid leukemia and in the management of ulcerative colitis (UC) and to provide appropriate results in treatment. Dasatinib is significantly higher and faster than full cytogenetic and large molecular responses as compared to imatinib.In the recent study, using the NMR data, thermochemical properties of the dasatinib structure, and the attached form of this molecule have been explored and analyzed. In this paper, we will examine some computational studies on this subject using semi-emperical and Monte Carlo methods. The Hyperchem 8.0 and Gaussian 09 and Gauss View 5 were used to do this. Methods for simulating molecular mechanics (MM+) and semi emperical. Quantum mechanics was calculated using B3LYP methods and the theoretical method of 6-31G. As a result, our findings indicate that the presence of Dasatinib can express the results of this molecule as anticancer agents.

کلمات کلیدی:

Dasatinib, NMR, Semi Empirical, Monte Carlo, Quantum Mechanics