عنوان مقاله:

Interaction of Vitamin B۳ with Parent Uracil and Anticancer Uracils: A Detailed Computational Approach

محل انتشار:

دوفصلنامه تحقیقات شیمی آلی, دوره 6, شماره 1 (سال: 1399)

تعداد صفحات اصل مقاله: 18

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خلاصه مقاله:

A detailed study on the formed complexes from interaction between vitamin B۳ with parent uracil and anticancer uracil's is performed using M۰۶-۲X/۶-۳۱۱++G(d,p) and B۳LYP/۶-۳۱۱++G(d,p) levels of theory. In the studied systems, the uracil's can be placed in three preferential interaction sites (A۱–A۳) in the vicinity of the vitamin B۳. For each uracil group, three configurations corresponding to energetic local minima are obtained. Among the various hydrogen bonding sites, the A۱ region of uracil's shows the strongest interactions at both levels of theory. The analyzed dimers are also stabilized by two hydrogen bonds (H-bonds). The predicted H-bonds in the formation of complexes are: O···H-N and O(S)···H-O. The topological properties of the electron density distribution are also analyzed in terms of the Quantum Theory of “Atoms in Molecules” (QTAIM). Furthermore, the natural bond orbital (NBO) analysis is applied to get a more precise insight about the nature of the H-bond interactions. The calculations reveal that, in most cases, the O(S)···H-O H-bonds are stronger than the O···H-N ones. The calculated energies of highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) show that charge transfer occurs within the molecules.

کلمات کلیدی:

Vitamin B۳, Anticancer uracils, DFT, NBO, QTAIM