Physical sorption between the molecule [4-(1,2,4-triazol-1-yl)-1-(2',3',5'-tri-O-acetyl-β-D-ribofuranyl)]uracil and CNT (12,12-8)

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Quantum chemistry seeks to accurately predict the chemical and physical properties of molecules and materials, useful in many fields and technology. Predicting chemical properties using an atomic scale approach is a theoretical and computational challenge. Quantum-chemical modeling of the spatial and electronic structure, physicochemical and chemical properties of known and atomic-molecular structures and their combinations is an effective method of chemical research. To carry out quantum-chemical calculations, computer facilities and quantum-chemical programs are needed, which are becoming more accessible and cheaper. The complexity of calculations is determined only by the atomic composition and the studied states of molecular systems. The calculations were performed using the ChemOffice 2016, Nanotube modeller, HyperChem 08, and Gaussian 09W software packages. During the work, we managed to find an energetically favourable complex between [4-(1,2,4-triazol-1-yl)-1-(2',3',5'-tri-O-acetyl-β-D-ribofuranosyl)] uracil and nanotube CNT (12,12-8).

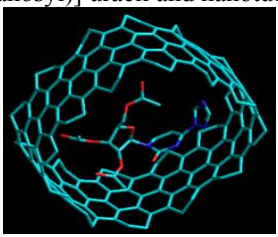

Fig. Complex between [4-(1,2,4-triazol-1-yl)-1-(2',3',5'-tri-O-acetyl-β-D-ribofuranosyl)] uracil and nanotube CNT (12.12-8)

The energies of the CNT (12,12-8) nanotube and the structural analogue of the pyrimidine nucleoside are 129.8 kcal/mol and 126.5 kcal/mol, respectively, that shows the stability of the system. Based on the data obtained, it can be assumed that the nanotube can theoretically act as a transfer agent, thereby having a high chance of penetration of a drug compound into diseased cells.

References

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