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Satyabrata Maiti et al., J Phys Chem Biophys 2018, Volume 8
DOI: 10.4172/2161-0398-C3-035

5th International Conference on
Physical and Theoretical Chemistry
October 11- 13, 2018 | Edinburgh, Scotland

Prediction of structures of dinucleotide steps containing non Watson-Crick base pairs

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Modern biology has unraveled that RNA can perform post-transcriptional gene regulation and many other functions. These are carried out by specific three-dimensional folded structures consisting of double helices mediated by Watson-Crick as well as various types of stable non Watson-Crick base pairs. Stacking interaction, which involves π electron delocalization, is most important for double helical structure. Hence we have studied such interactions using high level quantum chemical method (DFT-D) for various stacking geometries for two most frequently observed dinucleotide base pair step sequences containing G:A S:HT non Watson-Crick base pair. It was observed that the geometries corresponding to best stacking energy do not correspond to the experimentally observed geometry, indicating sugar-phosphate has a role to control the geometry. We have combined the DFT-D stacking energy with coarse grain energy arising from stretching of backbone. The hybrid energies shows high stability to the crystallographically determined orientations. There are quite a few additional non Watson-Crick base pairs, such as A:A w:wC, which are not very frequently found but may have important role in molecular biology. This base pair, stabilized by N-H...N and a non-polar C-H...N hydrogen bonds, can have two types of geometries having positive or negative shearing with almost equal stability. Inspired by the agreement between hybrid DFT-D and experiments, we attempted to predict stable geometry of stacking between A:A w:wC and G:U W:WC. It was observed that the structure of A:A w:wC having positive shear value is incapable to form double helix with positive roll and twist with negative slide, the nature of A-form RNA. The structures with negative shear, however, are found to have reasonable stacking energy for appropriate values of roll, twist, etc. Thus, the rather weak base pair with stabilization energy of around -10.4 kcal/mol (while -35 kcal/mol for G:C W:WC base pair), can form double helix with favorable stacking energy.

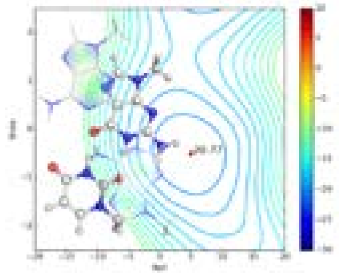

Figure 1: Representative figure for Stacking Energy contour of dinucleotide step sequence A:A w:wc::G:U W:WC.

Recent Publications:

1. Sarmistha Majumdar, Satyabrata Maiti and Subhra Ghosh Dastidar (2016) Dynamic and static water molecules complement the TN16 conformational heterogeneity inside the tubulin cavity. Biochemistry. 55(2):335-347.
2. Satyabrata Maiti and Dhananjay Bhattacharyya (2017) Stacking Interactions involving non-Watson-Crick base pairs: dispersion corrected density functional theory studies. Physical Chemistry Chemical Physics. 19(42):28718-28730.

Biography

Satyabrata Maiti started his research career as an experimental cum theoretical chemist. He used to synthesize target specific small molecules followed by basic theoretical calculation which was based on quantum chemical and docking study. He then moved to computational studies on proteins focusing on non bonding interaction between protein and ligand mediated by water molecules. He then joined in Saha Institute of Nuclear Physics, Kolkata for his doctoral research and working on computational studies on structure-function relationship of RNA.

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