Mapping the Intangible: Non-Covalent Forces Shaping Biological Structures and Functions

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ABSTRACT

Non-covalent interactions (NCI) are fundamental forces that stabilize molecular structures by preventing them from collapsing into disarray without the need for chemical bonds. These forces include van der Waals interactions, hydrogen bonds, electrostatic interactions, and hydrophobic effects. They are essential for maintaining the integrity and function of complex biological molecules such as proteins, DNA, and RNA, and play a central role in numerous biological processes. A critical function of non-covalent interactions is in solvation, where they influence the strength and specificity of solute-solvent interactions such that hydrogen bonds can stabilize a hydration shell around a solute, while van der Waals and hydrophobic interactions may encourage the aggregation of non-polar solute molecules in a solvent. The use of computational tools, notably the Reduced Density Gradient method a sophisticated means to visualize and analyze these interactions in detail within chemical systems. Together with Bader's Atoms In Molecule (AIM) theory, which utilizes electron density to delineate molecular boundaries and interactions, these tools offer robust methods for predicting and manipulating non-covalent interactions. Independent Gradient Model Based on Hirshfeld Partition, Local Energy Decomposition (LED), along with *Abinitio* Molecular Dynamics, can be used to enhance the understanding of the nature and dynamics of NCI more effectively.

This lecture will discuss various methods for analyzing non-covalent interactions between biomolecules and solvents, highlighting the utility of computational chemistry tools in probing these elusive yet crucial interactions taking Tapinarof-ethanol system as an example.

Reference

Jisha Mary Thomas and Renjith Thomas, Study of Non-Covalent Interactions Present in the Tapinarof–Ethanol System with Special Emphasis on Hydrogen-Bonding Interactions J. Phys. Chem. B 2023, 127, 26, 5933–5940