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Statistical Modeling Techniques for Unveiling Supramolecular Interactions

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Abstract: *Supramolecular interactions, the non-covalent forces that govern the assembly of molecules into complex structures, play a pivotal role in fields such as drug design, nanotechnology, and material science. Understanding these interactions requires an interdisciplinary approach combining experimental, theoretical, and computational methods. Among these, statistical modeling techniques have emerged as indispensable tools for decoding the intricate patterns and relationships underlying supramolecular systems. These techniques enable researchers to analyze experimental data, predict molecular behaviors, and uncover the fundamental principles driving supramolecular assembly. This paper explores the application of statistical modeling in elucidating supramolecular interactions, focusing on key methodologies, their advantages, and challenges, as well as emerging trends in the field.*

Keywords: Monte Carlo simulations, Docking studies, Quantum mechanical modeling, Force field analysis