Computer-Aided Formulation Design – A Paradigm Shift in Pharmaceutical Formulation Design

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Abstract

The escalating demand for innovative drug delivery methods has propelled the rigorous investigation and adoption of advanced computational methodologies, including machine learning and molecular simulation, within pharmaceutical research. Achieving a profound understanding of the intricate structure-property relationships that govern pharmaceutical formulation components is essential for accurately predicting their molecular-level behaviour.

This research focuses on critical areas such as chemical stability, reactivity, molecular degradation, impurity profiling, excipient selection, and precise crystal structure prediction of pharmaceutical ingredients. Furthermore, a comprehensive molecular elucidation of the Active Pharmaceutical Ingredient (API) is an indispensable prerequisite for initiating any robust formulation development process.

The Schrödinger simulation suites provide extensive computational workflows designed to predict and rigorously assess API behaviour under diverse conditions and in the presence of various excipients. This work will showcase compelling case studies that exemplify these advanced, molecular-level capabilities, demonstrating their utility in optimizing formulation design and accelerating the path to stable, efficacious drug products.