# Redefining Drug Discovery through Molecular Dynamics Simulations

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## ABSTRACT

Drug discovery has traditionally relied on chemical experiments and static molecular structures. In recent years, however**,** molecular dynamics (MD) simulations have emerged as a powerful computational tool that allows chemists to *see molecules in motion*. By simulating how atoms and molecules move and interact over time, MD provides a dynamic view of biological systems that cannot be captured by experiments alone.

This talk introduces the basic principles of molecular dynamics and explains how it is increasingly used in modern drug discovery. MD simulations help chemists understand how drugs bind to their targets, why some molecules are more stable or effective than others, and how small chemical changes can improve drug performance. Advances in computing, such as faster processors and GPU-based calculations, have made these simulations more accurate and accessible than ever before.

Through simple examples and selected case studies, in this presentation I will demonstrate how MD simulations connect chemical structure with molecular behavior. By moving beyond static pictures and embracing molecular motion, MD is helping chemists design better drugs in a more rational and efficient way.

**Keywords:** Molecular Dynamics (MD), Computational Chemistry, Drug Discovery, Molecular Motion, Protein–Ligand Interactions.

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