3. Pathgennie- Science & Technology

Ministry of Science and Technology develops software PathGennie for fast tracking of drug discovery The Ministry of Science and Technology introduced "PathGennie," an open-source software developed by the S.N. Bose National Centre for Basic Sciences to fast-track drug discovery. It efficiently simulates rare molecular events (like drug unbinding) using a "survival of the fittest" swarm simulation method, avoiding the artificial biases and high computational costs of traditional methods.

PathGennie- New Open-Source Software for Drug Discovery

Introduction and Overview

Launch Authority- The Ministry of Science and Technology has introduced this new tool to fast-track the drug discovery process.

Definition- PathGennie is a specialized software tool designed to simulate rare molecular events.

Core Function- It efficiently simulates complex processes such as A drug molecule unbinding (leaving) from a protein. Protein folding and unfolding transitions.

Developer- It was developed by scientists at the **S.**N. Bose National Centre for Basic Sciences in Kolkata, India.

Accessibility- The tool has been released as open-source software, making it freely accessible to the global scientific community to foster collaboration and innovation.

The Core Problem in Drug Development

The "Residence Time" Challenge- A critical factor in drug effectiveness is "residence time"—essentially, how long a drug stays bound to its target protein.

The "Rare Event" Obstacle- The process of a drug unbinding is considered a "rare event" in molecular terms. It occurs over timescales ranging from milliseconds to seconds.

Computational Limitations- Observing these events directly using standard molecular dynamics simulations is computationally impossible, even when utilizing powerful supercomputers, due to the vast time difference between atomic vibrations (femtoseconds) and unbinding events (seconds).

Comparison- Traditional Methods vs. PathGennie Approach

Feature	Traditional Simulation Methods	PathGennie Approach
Methodology	Uses artificial forces or high temperatures to force the unbinding event to happen within simulation time limits.	Launches swarms of ultra-short, unbiased simulations (only a few femtoseconds long) without forcing the molecules.
Physics Accuracy	Often distorts natural physics due to the external force applied.	Preserves true kinetics and natural physics by avoiding artificial biasing.
Prediction Quality	Can lead to potentially inaccurate predictions regarding how the drug behaves in reality.	Maps out transition pathways accurately, ensuring physically realistic results.

Operational Mechanism- PathGennie Works

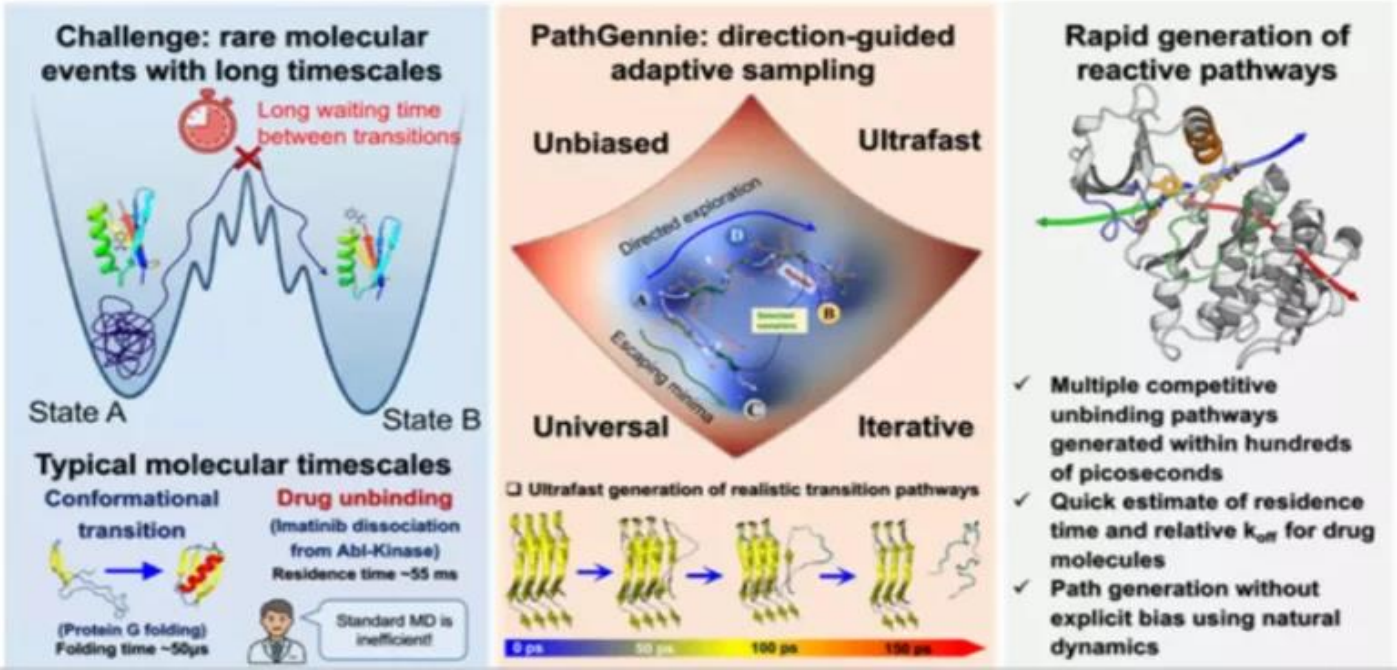
Swarm Intelligence- Instead of running one long simulation, PathGennie initiates a massive "swarm" of very short simulations.

Survival of the Fittest- It monitors these short simulation snippets. It selectively extends only those snippets that show progress toward the desired outcome (e.g., the drug moving away from the protein).

Unbiased Mapping- This strategy allows the software to efficiently map out the transition pathways based on probability and progress, without needing to artificially push the molecules.

Key Advantages

No Artificial Forces- Unlike traditional methods that rely on external biases or elevated temperatures, PathGennie ensures physically realistic pathways.



Rapid Pathway Discovery- By balancing "exploration" (trying new paths) and "exploitation" (following promising paths), it quickly identifies multiple possible pathways for rare events that would otherwise require prohibitively long simulation times.

Flexible and General-Purpose- The algorithm is adaptable to a wide range of problems. It can operate using any set of collective variables (parameters describing molecular progress). It handles high-dimensional variables, making it versatile for complex systems.

Wider Applications

PathGennie is not limited to drug discovery; it is a general-purpose framework applicable to various rare molecular events, including

1. Chemical Reactions- Understanding reaction pathways.
2. Catalytic Processes- Improving efficiency in industrial catalysis.
3. Phase Transitions- Studying changes in states of matter.
4. Self-Assembly Phenomena- Understanding how molecules organize themselves.
5. AI Integration**-** The software is compatible with machine-learning techniques, allowing researchers to use parameters learned by Artificial Intelligence to further guide and refine the simulations.

Source- https-//www.newsonair.gov.in/ministry-of-science-and-technology-develops-software-pathgennie-for-fast-tracking-of-drug-discovery/