

PathGennie

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PathGennie Latest News

Recently, the Ministry of Science and Technology has developed new open-source software called PathGennie.

About PathGennie

- It is a **novel computational framework** developed by scientists that can significantly accelerate the simulation of **rare molecular events**.
- It is **open source software** developed for **fast tracking of drug discovery**.
- It is aimed at **fast-tracking the drug discovery** process by accurately tracking molecular unbinding pathways.
- It addresses a long-standing challenge in **molecular simulations** — accurately modelling how drug molecules detach from their target proteins.
 - This process, known as **ligand unbinding**, plays a key role in determining a drug's "residence time", which is often more relevant to therapeutic effectiveness than binding strength alone.

- It predicts the **potential drugs unbind** from their protein targets without the artificial distortions commonly used in standard methods.
- It mimics **natural selection** on a microscopic scale **instead of forcing the molecule to move**.

Features of PathGennie

- It **captures rare molecular** events without artificial acceleration.
- It generates multiple competitive unbinding pathways.
- It estimates residence time of drug molecules.
- It eliminates bias introduced by external force-based simulations

Potential Applications of PathGennie

- It addresses problems such as **chemical reactions, catalytic processes**, phase transitions, or self-assembly phenomena.
- It is also **compatible with modern machine-learning techniques** which ensures integration into **diverse simulation pipelines**.

Source: **News On Air**

Source: <https://vajiramandravi.com/current-affairs/pathgennie/>

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