PathGennie: Open-Source Drug Discovery

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In the News: The Ministry of Science and Technology (via the **S.N. Bose National Centre, Kolkata**) launched **PathGennie**, an open-source software designed to accelerate drug discovery.

Technological Innovation

- **Molecular Dynamics:** It uses a "direction-guided adaptive sampling" algorithm to simulate **rare molecular events**, such as how a drug molecule unbinds from a protein target.
- **Survival of the Fittest:** Instead of using "artificial force" to speed up simulations (which can distort data), PathGennie launches thousands of short "scouting" missions and only extends those that show progress.

Strategic Utility

- **Fast-tracking Pharma:** It reduces the time needed to predict a drug's **"residence time"** (how long it stays attached to a target), which is a key factor in drug efficacy.
- **Open-Source Paradigm:** By being open-source, it allows Indian MSMEs and researchers to bypass expensive proprietary software, supporting the **'Atmanirbhar Bharat'** in pharmaceuticals.