

Accelerating Pharmaceutical Innovation

Leveraging AI and Platform Engineering to Revolutionize Drug Development



Amit Taneja

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Traditional Drug Discovery Challenges

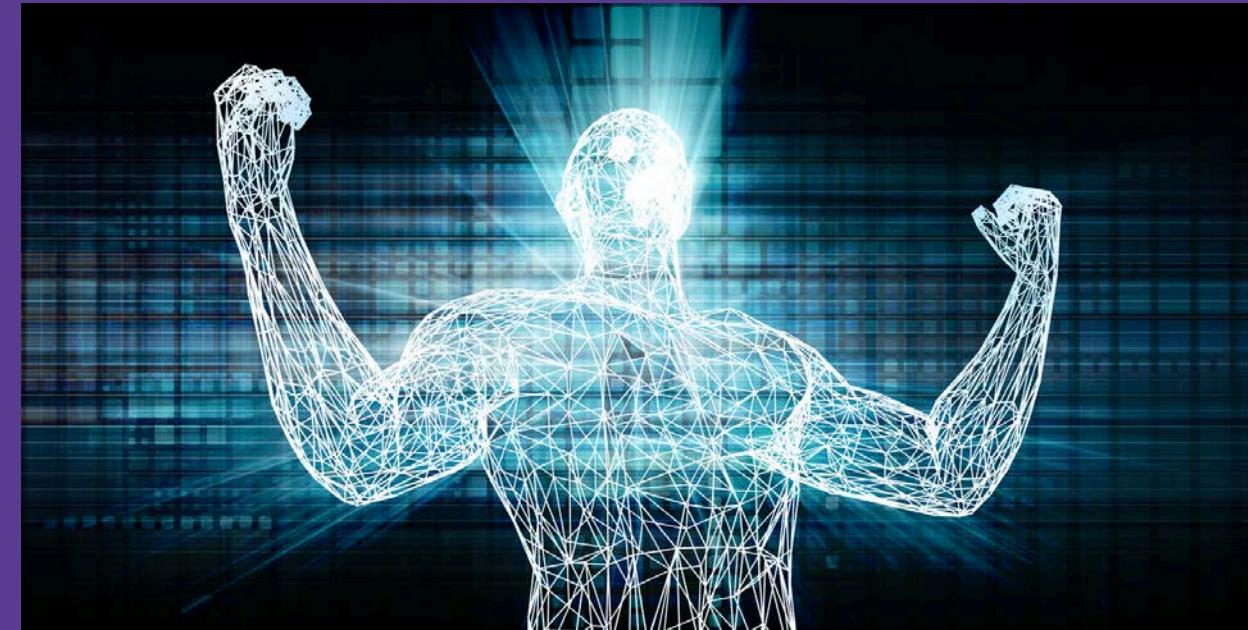
- **High Costs:** The average cost to develop a new drug exceeds \$2.6 billion.
- **Long Timelines:** On average, it takes 12+ years to develop and approve a new drug.
- **Inefficiency:** Traditional methods rely on experimental screening, which is time-consuming and costly.



Automating Workflows with Platform Engineering

- By automating workflows using platform engineering practices, we can streamline drug discovery processes, reduce manual intervention, and improve operational efficiency. Automated pipelines ensure data moves seamlessly from one phase to another, saving time and resources.

AI's Transformative Role in Drug Discovery



- AI provides faster data analysis, identifying promising drug candidates with higher efficiency.
- AI-powered solutions predict molecular interactions, reducing drug discovery time.
- AI improves accuracy, with models predicting success rates over 80%.

Scalable Cloud Infrastructure in Platform Engineering

- Platform engineering enables scalable cloud infrastructure that supports AI models in processing large datasets, optimizing compute resources, and reducing time for molecular analysis. Scalable systems ensure that AI processes grow dynamically with project needs, eliminating bottlenecks.

AI Methodologies in Drug Discovery

- **Deep Learning:** Models like CNNs and RNNs analyze chemical and bioactivity data.
- **Virtual Screening:** AI evaluates large chemical libraries, identifying high-potential compounds.
- **Molecular Docking:** AI simulates molecular interactions, predicting how drugs will bind to targets.
- **Generative Models:** AI creates novel molecules for specific therapeutic purposes.



Continuous Integration and Deployment (CI/CD) in Platform Engineering

- Using CI/CD principles, platform engineering automates the deployment of AI models, ensuring that every iteration or improvement is quickly tested and integrated. This speeds up the time between model training, testing, and deployment, reducing downtime and manual intervention.

Case Study 1 – AI-Driven Molecule Discovery

Exscientia & Sumitomo Dainippon Pharma:

- AI created a molecule for immuno-oncology, reducing the development timeline to just 8 months.
- Entered clinical trials faster than traditional timelines (typically 4-5 years).
- Highlights AI's ability to expedite the discovery process.

Faster Time-to-Market with Platform Engineering

- Platform engineering practices played a key role in speeding up the time-to-market for the AI-designed molecule. By automating key processes, handling large datasets, and integrating various research tools, the entire drug discovery timeline was significantly shortened.

Case Study 2 – AI-Discovered Antibiotic

Halicin Discovery

- AI screened over 6,000 compounds and identified Halicin, an antibiotic effective against drug-resistant bacteria.
- Halicin exhibited a novel mechanism of action, targeting ATP synthase.
- Demonstrated AI's ability to find innovative therapeutic solutions.

Data-Oriented Architecture in Platform Engineering

- In the case of Halicin, platform engineering provided a data-oriented architecture that enabled the AI models to handle, process, and analyze vast datasets. By centralizing data pipelines, the AI was able to screen compounds more efficiently and accurately.

The Benefits of AI in Drug Discovery

- **Reduced Time:** AI dramatically shortens drug development timelines.
- **Lower Costs:** Fewer trials and errors reduce development expenses.
- **Higher Accuracy:** AI predictions significantly increase the chances of success for compounds.



Optimizing Resources with Platform Engineering

- Platform engineering ensures that resources—both computational and financial—are optimized. It allows for the automatic scaling of compute power and storage based on AI model demands, ensuring efficient use of resources without unnecessary cost increases.

Challenges and Considerations



- **Data Quality:** AI relies on large datasets that must be accurate and comprehensive.
- **Model Interpretability:** Complex AI models can be difficult to understand and interpret.
- **Experimental Validation:** AI predictions must still undergo rigorous experimental validation.

Observability and Monitoring in Platform Engineering

- Platform engineering emphasizes observability and monitoring tools that help track data flow and model performance. These tools make it easier to detect issues in AI models, ensuring higher accuracy and quality of the data used in drug discovery.

Future Outlook for AI in Drug Discovery

- **Next-Generation AI Tools:** Advanced models will further accelerate the discovery process.
- **Collaboration:** Partnerships between AI experts, chemists, and biologists will drive innovation.
- **Expansion:** AI will help develop personalized medicine and targeted therapies.



Collaboration Platforms with Platform Engineering

- In the future, platform engineering will facilitate better collaboration between interdisciplinary teams by creating integrated environments where data scientists, biologists, and chemists can work together on drug discovery. These platforms will streamline communication and data sharing.

Conclusion

Artificial intelligence has the potential to revolutionize the pharmaceutical industry by accelerating drug discovery processes, improving accuracy, and significantly reducing costs.

As AI-driven approaches continue to evolve, they offer new possibilities for identifying promising drug candidates, predicting molecular interactions, and optimizing drug formulations. However, the success of AI in drug discovery is heavily dependent on robust platform engineering.



THANK YOU