Digital Transformation in Pharma R&D: How AI/ML, Chemical-Space Docking, FEP, and Emerging In Silico Methods are Improving Success Rates in Drug Discovery

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Abstract

Drug discovery is entering a new era of AI, machine learning, and digital innovation, where advanced *in silico* methodologies are accelerating timelines, reducing costs, and improving success rates.

Recent developments include:

- **Chemical-Space Docking,** enabling the screening of billions to trillions of molecules with hit rates approaching 40%.
- **Free Energy Perturbation (FEP),** delivering accurate binding affinity predictions for small molecules, peptides, and diverse targets within hours.
- **Polymorphism prediction,** now achieving up to 98% accuracy.
- **AI/ML-driven formulation design,** tackling solubility and stability challenges with ~85% predictive accuracy.
- Computation of 200+ ADMET properties, high-throughput PBPK simulations, and early pKa predictions to prevent late-stage attrition.
- **AI/ML + literature-based retrosynthesis tools,** transforming synthetic route design, process chemistry, and impurity prediction.
- **Large Language Models (LLMs), Generative AI,** and AI-driven atomistic simulations, expanding the scope of digital drug design and development.

Together, these innovations are reshaping the drug discovery paradigm, enhancing hit identification, lead optimization, and translational outcomes.

Yet, many academic and research institutes continue to rely heavily on traditional methods, missing opportunities to harness these advances. This presentation will:

1. **Explain the methodology and science behind these emerging approaches.**

2. **Highlight real-world case studies demonstrating measurable impact.**

Share actionable strategies for institutions to adopt digital drug discovery and remain competitive in the evolving R&D landscape.