



Pi-AlphaFold Drug Discovery (Pi-AFDD)



Technological advancements in data and artificial intelligence are redefining the way a drug is discovered.

There is a need for a comprehensive and user-friendly solution that combines advanced AI models with other tools for protein analysis and drug discovery.

Many BioPharma companies do not have the specialized skills and large computational resources that are needed to use advanced AI models like AlphaFold2.

Persistent Systems’s Pi-AFDD workbench with integrating AI models and computational tools unlock opportunities in drug discovery.

Integration of AlphaFold2 and AutoDock allow protein structure prediction and virtual screening of large libraries of molecules to quickly discovery hit compounds.

Interactive KG with Google LLM help to analyze complex biomedical data to identify drug targets with biological insights.

Smart Report Builder allows to capture critical data from the workflow and create smart reports with Google LLM.

Pi-AFDD

Pi-AFDD is designed to enhance the efficiency and accuracy of several critical steps in early drug discovery, such as target identification, protein structure prediction, and hit / lead discovery.

Pi-AFDD offers a user-friendly interface that accelerates early drug discovery by integrating advanced AI and GenAI models with computational tools.

Current applications include target identification with insights, 3D protein structure prediction, binding site prediction, virtual screening, and smart documentation, thereby saving time and costs in discovering hit molecules.

Traditional methods of drug discovery and development are lengthy, expensive and labor-intensive.



Manual workflows

Drug discovery is an expensive, multi-step and time-consuming processes.



Low success rate to market

On average 1 molecule get FDA approved out of 10000 molecules.



Legacy digitization infrastructure

Limited compute resources for digitizing drug discovery workflow.

Pi-AlphaFold Drug Discovery (Pi-AFDD) works in three phases

Phase 1: Target Discovery

Discover novel targets against a disease with GenAI powered KG

Complex Data Mining with Knowledge Graph

Import diverse relationship data and visualize with GenAI powered KG

Draw Biological Insights

Analyzes literature and proprietary documents to streamline target prioritization

KG with GCP LLM Models

Integrates KG, KG ChatBot, and BioInsight ChatBot for seamless target discovery

Phase 2: Hit Identification and Lead Optimization

Generate protein structure, screen chemical library, optimize lead molecules

Protein Structure and Binding Site Predictions

Predict structure of the target protein and ligand binding site using AlphaFold2 and Fpocket

Discover Hit Molecules

Screen molecule libraries using molecular docking tools

Optimize Lead Compounds

Optimize leads with structure-based approach and similarity search

Phase 3: Smart Report Builder

Organize data and generate smart reports

Workflow Drafts

Capture crucial steps of workflow as drafts and generate smart reports enriched by GCP LLM

Automated Report Generation

Leverages GCP GenAI to streamline the creation of comprehensive reports

Time and Cost Efficiency

Significantly reduces the time and effort required to document the drug discovery process

Why Pi-AFDD?

Accelerated Drug Discovery

Pi-AFDD uses AI and computational tools to speed up target identification, protein structure prediction, and hit / lead discovery, reducing time to market for new drugs.

Efficiency with Higher Success Rate

Combining advanced AI models with computational tools, Pi-AFDD ensures fast and accurate drug discovery, improving success rates for pharma and biotech sectors.

Advanced AI and Computational Tools

Utilizing AI models like AlphaFold2, Gemini, Vertex AI, and tools like AutoDock, Pi-AFDD offers a flexible solution for early drug discovery needs.

Flexible and Scalable

The workflow adapts to industry-specific demands and can be implemented on client premises or hyperscalers, suitable for the pharma, biotech, and biopharma sectors.

Start your Pi-AFDD journey today. Reach out to a specialist to identify next steps.

Contact Us

About Persistent

Persistent Systems (BSE & NSE: PERSISTENT) is a global services and solutions company delivering Digital Engineering and Enterprise Modernization to businesses across industries. With over 23,900 employees located in 19 countries, the Company is committed to innovation and client success. Persistent offers a comprehensive suite of services, including AI-enabled software engineering, product development, data and analytics, CX transformation, cloud computing, and intelligent automation. The Company is part of the MSCI India Index and is included in key indices of the National Stock Exchange of India, including the Nifty Midcap 50, Nifty IT, and Nifty MidCap Liquid 15 as well as several on the BSE such as the S&P BSE 100 and S&P BSE SENSEX Next 50. Persistent is also a constituent of the Dow Jones Sustainability World Index. The Company has achieved carbon neutrality, reinforcing its commitment to sustainability and responsible business practices. As a participant of the United Nations Global Compact, Persistent is committed to aligning strategies and operations with universal principles on human rights, labor, environment, and anti-corruption, as well as take actions that advance societal goals. With 327% growth in brand value since 2020, Persistent is the fastest-growing IT services brand in the 2024 Brand Finance India 100 Report.

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