MolecuLayer: A Decentralized Compute Marketplace for Drug Discovery

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Abstract

MolecuLayer is a decentralized blockchain protocol that revolutionizes drug discovery by enabling a peer-to-peer marketplace for machine learning inference and validation. By leveraging distributed GPU resources, MolecuLayer allows miners to process complex drug discovery prompts, validators to ensure solution quality, and researchers to access cutting edge computational tools at reduced costs. Powered by the native MLYR token, MolecuLayer democratizes access to advanced AI-driven drug discovery, fostering innovation and collaboration in a transparent, secure, and community-driven ecosystem.

1 Introduction

The pharmaceutical industry faces significant challenges in drug discovery, including high computational costs, centralized control of AI tools, and barriers to accessing diverse datasets and models. Traditional drug discovery pipelines rely on proprietary software and expensive infrastructure, limiting participation to well-funded organizations. Meanwhile, advances in AI, such as AlphaFold and molecular docking simulations, have demonstrated the potential to accelerate drug discovery, but these tools remain inaccessible to many researchers.

MolecuLayer addresses these challenges by creating a decentralized compute marketplace tailored to drug discovery. Inspired by projects like Bittensor and Arbius, MolecuLayer enables GPU operators (miners) to process drug discovery prompts, validators to verify solutions, and researchers to submit complex queries, all within a blockchain-based ecosystem. The native MLYR token incentivizes participation, ensures quality, and facilitates transactions. This whitepaper outlines MolecuLayer's vision, technical architecture, tokenomics, and roadmap.

2 Problem Statement

Drug discovery is a resource-intensive process, with computational costs often exceeding millions of dollars per project. Key challenges include:

- High Costs: Proprietary AI tools and high-performance computing infrastructure are prohibitively expensive for small research groups.
- Centralized Control: Centralized platforms limit access to advanced models and datasets, stifling innovation.
- Validation Bottlenecks: Ensuring the accuracy of AI-generated molecules requires expert validation, which is time-consuming and costly.
- Data Privacy: Researchers hesitate to share proprietary prompts or datasets due to intellectual property concerns.

MolecuLayer solves these problems by decentralizing compute resources, incentivizing quality through token rewards, and providing a transparent validation mechanism.

3 Architecture

3.1 Participants

MolecuLayer involves three participant groups:

- Miners: GPU operators (e.g., A100, H100, or retail GPUs) who process drug discovery prompts off-chain using AI models of their choice. A default open-source model is provided for accessibility.
- Validators: GPU operators who verify the accuracy of miners' solutions. All miners can optionally validate, sharing a portion of mining rewards.
- Researchers: Users who submit prompts (e.g., plaintext or 3D molecule files) and deposit bids in MLYR tokens or other cryptocurrencies.

3.2 Workflow

1. Researchers submit prompts to the MolecuLayer smart contract, specifying requirements (e.g., receptor selectivity, EC50 thresholds) and a bid.
2. Miners retrieve prompts, process them off-chain using AI models, and submit solutions on-chain.
3. Validators review solutions during a 6-hour optimistic validation window. Solutions are assumed valid unless rejected.
4. The system periodically injects invalid solutions to test validator diligence. Validators failing to reject invalid solutions face penalties.
5. Valid solutions trigger reward distribution in MLYR tokens to miners and validators.

3.3 Technical Components

- Blockchain: MolecuLayer operates on the Ethereum Layer-2 chain Base for low transaction fees.
- Smart Contracts: Handle prompt submission, solution hash storage, validation, and reward distribution.
- Off-Chain Compute: Miners and validators perform inference and validation off-chain to reduce blockchain load.

4 Tokenomics

The MLYR token is the native cryptocurrency of MolecuLayer, with a maximum supply of 50 million tokens and a 4-year halving cycle. Key functions include:

- Rewards: Miners and validators earn MLYR tokens based on solution quality and validation accuracy.
- Bids: Researchers deposit MLYR tokens (or other cryptocurrencies with a higher system fee) to incentivize miners.
- Governance: Token holders vote on protocol upgrades and validator penalties.
- Staking: Validators stake MLYR tokens to participate, with slashing for malicious behavior.

4.1 Token Distribution

- 40%: Mining and validation rewards
- 20%: Ecosystem development
- 15%: Team and advisors

- 15%: Community and marketing
- 10%: Initial liquidity

4.2 Fee Structure
- Native MLYR bids: 5% system fee
- Non-native token bids: 10% system fee

5 Incentive Mechanisms

MolecuLayer uses cryptoeconomic incentives to ensure quality and participation:
- Miners: Compete to provide the best solutions, with rewards proportional to solution quality (e.g., docking scores, selectivity metrics).
- Validators: Earn a share of mining rewards for accurate validation. Periodic invalid solution tests penalize negligence.
- Researchers: Higher bids attract more miners, increasing the likelihood of high-quality solutions.

6 Roadmap

- Q3 2025: Testnet launch with basic prompt processing and validation. • Q1 2026: Mainnet launch with support for plaintext and 3D molecule prompts.
- Q3 2026: Integration of advanced models (e.g., AlphaFold derivatives) and governance features.
- Q1 2027: Expansion to other scientific compute tasks (e.g., protein folding, material science).

7 Conclusion

MolecuLayer pioneers a decentralized approach to drug discovery, empowering researchers, GPU operators, and validators to collaborate in a transparent and incentivized ecosystem. By leveraging blockchain technology and AI, MolecuLayer reduces costs, democratizes access, and accelerates innovation in one of humanity's most critical fields. Join us in building the future of decentralized science.

8 References

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