FOR IMMEDIATE RELEASE

CIPHERICA Launches CIPHER-SKI: The LLVM of Drug Discovery

Revolutionary "Molecular Compiler" Treats Molecules Like Computer Programs

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CIPHERICA today announced the launch of CIPHER-SKI (patent pending), a groundbreaking AI platform that fundamentally rewrites chemistry with intelligence to accelerate drug discovery.

CIPHER-SKI is not another generative model. It is the LLVM of drug discovery, a complete molecular compiler that treats every molecule like an executable computer program. It takes simple fragments and intelligently rewrites them into optimized, drug-like candidates using the same principles that power today's most advanced compilers.

"CIPHER-SKI is not a generative model. It is the LLVM of drug discovery, a full compiler stack whose source language is chemistry, whose target language is biologically active, topologically rich, drug-like molecules, and whose optimization objective is 'maximize interesting 3D structure + therapeutic utility'." — Gershon Wolfe, Ph.D., Founder of CIPHERICA

CIPHER-SKI's neuro-symbolic dual-evolution engine fuses deep neural networks with symbolic reasoning. It operates in two phases that mirror real medicinal chemistry:

1. **Smart Scaffold Hopping:** Energy-guided graph rewriting using persistent homology to create rich 3D character (spiro rings, bridged systems, cavities).
2. **Branch Optimization:** Adding clinically proven side chains while balancing binding affinity, ADME, QED, and synthetic accessibility. The system learns from every run, remembering high-performing cores while retaining the ability to make bold jumps.

Why This Matters

While most AI platforms only decorate known scaffolds with incremental changes, CIPHER-SKI operates as a true molecular compiler. Just as functional programming reduces complex expressions through successive term rewrites, CIPHER-SKI applies formal term graph rewriting (Double Pushout style) to molecular graphs, performing energy-guided scaffold hops followed by branch optimization. This systematically reduces the search space while ensuring chemical validity and synthetic accessibility, yielding genuinely novel molecules with distinctive "spiro-rich, bridged, 3D" character. Recent highlights include PROTACs achieving an exceptional -13.9 kcal/mol docking score with textbook ternary geometry on EphB1, and KRAS G12C scaffolds reaching -11.1 kcal/mol — matching or exceeding performance reported by leading internal Big Pharma de novo platforms.

Formal Term Graph Rewriting Engine (Clinical Warhead Edition)

CIPHER-SKI contains a powerful Formal Term Graph Rewriter; a Double Pushout symbolic rewriting system that applies clinically validated rewrite rules. For example, this engine automatically injects rigid spiro[3.3]heptane and bicyclo[1.1.1]pentane linkers, the signature

piperidine-methyl-piperazine rigid motif widely used in advanced oral AR and ER degraders, 6-fluoro-isoindolinone CRBN warheads, trans-1,4-cyclohexyl and pyridazine-carboxamide connectors from clinical PROTACs, VHL hydroxyproline/tert-butyl attachments, and precise warhead-to-linker/E3 attachment points that have enabled oral bioavailability and high potency in late-stage programs. The result: PROTAC chimeras that are genuinely drug-like, synthetically tractable, and optimized for ternary complex geometry.

Key Highlights

- Neuro-symbolic dual-evolution architecture with intelligent memory
- Energy-guided scaffold hopping via persistent homology
- Fully explainable, transparent decision-making
- 3D topology-aware evaluation
- Intelligent multi-parameter optimization (binding + ADME + QED + developability)
- Dedicated PROTAC mode with 50+ clinical rewrite rules

About CIPHER-SKI & CIPHERICA

CIPHER-SKI (patent pending) was developed by CIPHERICA, an AI-first biotechnology company building hybrid neuro-symbolic platforms to solve previously intractable challenges in drug discovery. The platform combines intelligent graph rewriting, reinforcement learning, and advanced 3D topological analysis into a clean two-phase system that separates core innovation from side-chain optimization.

CIPHERICA is actively engaging with strategic partners to advance CIPHER-SKI across multiple therapeutic areas.

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