AI/Computational Platform

CANDDIE™ | AI/MD Drug Discovery Platform for Challenging Membrane Protein Targets

Membrane Protein Modeling • Binding Affinity & Signaling Prediction • CADD Automation

Atomatrix

Technology Summary

Atomatrix is a computational drug discovery company specializing in AI- and molecular dynamics (MD)-based modeling and simulation for challenging membrane-protein targets, including GPCRs. Its proprietary CANDDIE™ platform integrates three core capabilities: membrane-protein modeling, MD-based binding affinity and downstream signaling prediction, and AI/MD-driven CADD automation.

Together, these capabilities extend conventional structure-based CADD beyond static binding assessment toward membrane-aware dynamic evaluation and mechanism-oriented analysis, providing deeper insights to support compound prioritization, lead optimization, and drug discovery decision-making.

Atomatrix currently provides paid, target-specific B2B drug discovery services and is productizing CANDDIE as a cloud-based SaaS platform to make advanced computational drug discovery capacities more broadly accessible to pharmaceutical and biotechnology companies worldwide.

Core Technology Strengths

1 | AI/MD-Based Membrane Protein Modeling

- PDB- and AlphaFold-based structure refinement
- Membrane-aware system preparation for GPCRs and other challenging membrane targets
- Drug-design-ready structural models incorporating target conformational state, protein flexibility, and membrane environment.

2 | Binding Affinity & Signaling Prediction

- Baron™: MD-based binding affinity prediction and ligand stability assessment
- Allopiper™: ligand-induced allosteric communication and signaling-related structural conformational changes
- Mechanistic interpretation of ligand binding and signaling beyond static docking scores

3 | AI/MD-Driven CADD Automation

- Automated target and ligand preparation, docking, MD, Post-MD analysis, and reporting
- End-to-end CADD workflows for globular and membrane-protein targets.
- Cloud-based SaaS deployment reducing the need for in-house MD expertise and GPU infrastructure.

~~High Value~~ Drug-Design Use Cases

Incomplete Target Structures

When experimental structures are incomplete, the relevant conformational state is uncertain, or the membrane environment affects target structure and dynamics.

Membrane-aware system preparation

Candidate Prioritization after Docking

When structurally related compounds show similar docking poses or scores and require further evaluation of binding stability and relative affinity.

MD + BARon™

Mechanism-Driven Differentiation

When compounds with comparable binding affinity in biased agonism, allosteric modulation, or downstream signaling.

Allopiper™

CANDDIE connects target structure, dynamic binding behavior, and downstream signaling within an automated workflow to support compound prioritization and optimization.

Computational Automation for New Drug Discovery with Intelligent Experimentation

Post-MD Analysis Engines | BARon™ & Allopiper™

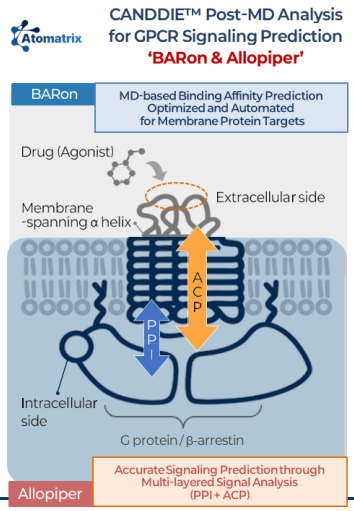
BARon™ | MD-Based Binding Affinity & Stability Prediction

BARon analyzes MD trajectories to evaluate ligand-target energetics and binding stability, supporting relative binding-affinity ranking when docking scores provide limited separation.

Allopiper™ | Allostery & Signaling-related Analysis

Allopiper analyzes ligand-induced conformational change and allosteric communication associated with downstream signaling. For GPCR programs, it provides mechanistic analysis of signaling selectivity, biased agonism, and allosteric modulation.

Both modules are computational decision-support tools intended to complement, not replace, experimental validation.



Scientific Foundation, Project Results & Commercial Traction

Scientific Foundation	Project-Specific Results	Commercial Traction
• 13 SCI-indexed publications in CADD, MD, and related computational methodologies • 3 publications in 2025, including a *Chemical Science* Hot Article • Research spanning GPCRs and other protein target classes	• Oncology program: 272 of 424 compounds met project-defined hit criteria • Dual-target metabolic program including GLP-1R: 2 of 8 compounds met project-defined hit criteria • Results are specific compound sets and hit criteria for each project	• Paid CANDDIE-based drug-design projects with three Korean pharmaceutical and biotechnology companies in 2026 • Project outcomes and user feedback are incorporated into computational protocols, algorithms, and workflow development

** Project-specific results should not be interpreted as representing the overall predictive accuracy of the CANDDIE platform.*

Technology Infrastructure & Product Development

Membrane-Aware Modeling & System Preparation PDB- and AlphaFold-based structure refinement, missing-region reconstruction, and membrane system preparation with target-specific compositions for GPCRs and other membrane protein targets.	**Screening & Docking Infrastructure** Virtual-screening resources covering >1 billion compounds, with in-house compound filtering and multiple docking approaches for chemical-space exploration and candidate prioritization.
Automated Molecular Dynamics Automated system construction, solvation and membrane setup, equilibration, MD simulation, and post-MD analysis for both globular and membrane protein systems.	**SaaS Product Development** Working CANDDIE SaaS prototype built on an Azure-centered cloud architecture for GPU computing, data isolation, and role-based control.

IP & Brand Protection

- Core CANDDIE technology: Korean patent application filed
- CANDDIE brand: two Korean trademark applications filed

Scientific Evidence & External Recognition

- 13 SCI-indexed publications; selected evidence includes *Chemical Science* (2025), *Journal of Molecular Graphics and Modeling* (2023), and *Nature Communication* (2022)
- Selected for Korea's TIPS R&D program and a Microsoft collaboration program

** Project-specific performance results and computational predictions are intended to support research decisions and require experimental validation. IP development is ongoing alongside CANDDIE platform development.*

ATOMATRIX | PARTNERSHIP & COMMERCIALIZATION

How We Can Work Together

Atomatrix can complement a partner's existing CADD and experimental workflows or provide an integrated computational workflow. New engagements typically begin with a defined target, compound set, and project objective, with scope expanded based on project results and partner needs.

1 | Pilot / Feasibility Study	2 | Target-Specific B2B project	3 | Computational–Experimental collaboration	4 | Joint Discovery Program
Defined target and compound set Technical feasibility and workflow fit	Paid project with defined scope, milestones, and deliverables. Hit identification and lead optimization	CANDDIE analysis combined with partner and CRO experimental assays Iterative evaluation and hypothesis refinement	Longer-term discovery or co-development collaboration Commercial terms defined on a case-by-case

Typical Project Workflow | From Client Inputs to Project Outputs

Client Inputs

- Target sequence and available structure data
- Client-provided compound set or CANDDIE screening library
- Desired MoA and project-specific hit/lead selection criteria
- Available assay and pharmacology data, where applicable

CANDDIE Analysis Workflow

Target-specific application of the three CANDDIE technology pillars

Target Information	AI/MD-Based Target Modeling	Drug-Ready Library / DB	AI-Based Docking	MD-Based Prioritization

Automated MD / Post-MD Analysis

BARon™
Binding-affinity prediction and dynamic-stability assessment

Allopiper™
Allosteric and signaling-related analysis, when relevant

Project Outputs

- Prioritized candidate compounds
- Binding-affinity prediction and stability assessment / ranking
- MoA and signaling-related mechanistic analysis, where relevant
- Project report with recommendation for experimental follow-up

Commercialization Roadmap

AVAILABLE NOW	Q4 2026	Q1 2027+
Paid B2B Drug-Design Services **Pilot and target-specific projects**	**CANDDIE SaaS Beta** **Selected-user testing and workflow evaluation**	**CANDDIE SaaS Commercial launch** **Subscription-based access and expansion of global partnerships**

A typical relationship may progress from a pilot to a paid project, followed by SaaS adoption or a longer-term joint program, depending on project results and partner objectives.

Leadership & Contact

Eunho Lee, Ph.D. | Founder & CEO

• 27 years of expertise in small-molecule drug discovery, R&D leadership, and technology commercialization, including the management of multi-disciplinary drug-discovery programs.
• Co-inventor of XCOPRI® (cenobamate), an FDA-approved antiseizure drug, with experience spanning candidate discovery, lead development, and preclinical R&D.

Sangbae Lee, Ph.D. | VP & CTO

• 29 years of experience in CADD, molecular modeling, and MD-based drug design, including GPCR research at City of Hope and research on membrane protein structure, dynamics, and signaling.
• Leads the development of CANDDIE, including membrane protein modeling, automated MD workflows, BARon™ binding-affinity analysis, and Allopiper™ allostery signaling-related analysis.

Contact

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Leadership combining small molecule drug discovery and R&D commercialization with CADD, GPCR, molecular modeling, and computational platform-development.

We would welcome the opportunity to explore how CANDDIE™ could support your targets of interest or drug discovery programs through a non-confidential technical and business discussion.