# ADVANCED SOLUTIONS TO DRUG DISCOVERY

LNP Solution

# We Never Compete with Our Clients.

We use molecular modeling simulations and deep learning techniques to identify early Hit candidates in drug discovery, with optimized technology, experience, and confidence to drive success.
We are also building LNP AI Smart Bench that researchers can easily use throughout the drug discovery process, leveraging the latest in AI, deep learning, and big data technologies.

With us, you have the **best partner** for successful drug discovery.

## Molecular Modeling + AI = Novel Drug

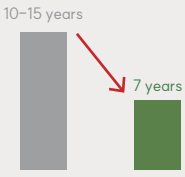
**CADD**
Molecular Modeling

**AI**
Artificial Intelligence

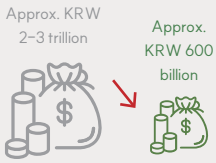
Compound design techniques based on protein structure

Compound ADME and toxicity prediction technology through deep learning model development

### The Advantages of Leveraging AI and Simulation in Drug Discovery




**Reduced development time**




**Reduced development costs**

**Candidate identification stage**

- Quickly browse over 1 million articles
- Minimize time and labor costs

**Clinical trial stage**

- Present drug candidates
- Identify optimal patient groups for clinical trials

Up to an 80% reduction in cost/time compared to traditional drug discovery process

# AI Screening **Solution**


Our molecular modeling and AI-powered analytics identify optimal molecules and provide solutions to make drug discovery faster, more efficient, and ultimately more successful.

| Research Service Business | | Platform Package Business |
|---|---|---|
| Research Service | Collaborative Research | AI-CADD based analysis Package & Web Service |

### ◎ Research Service

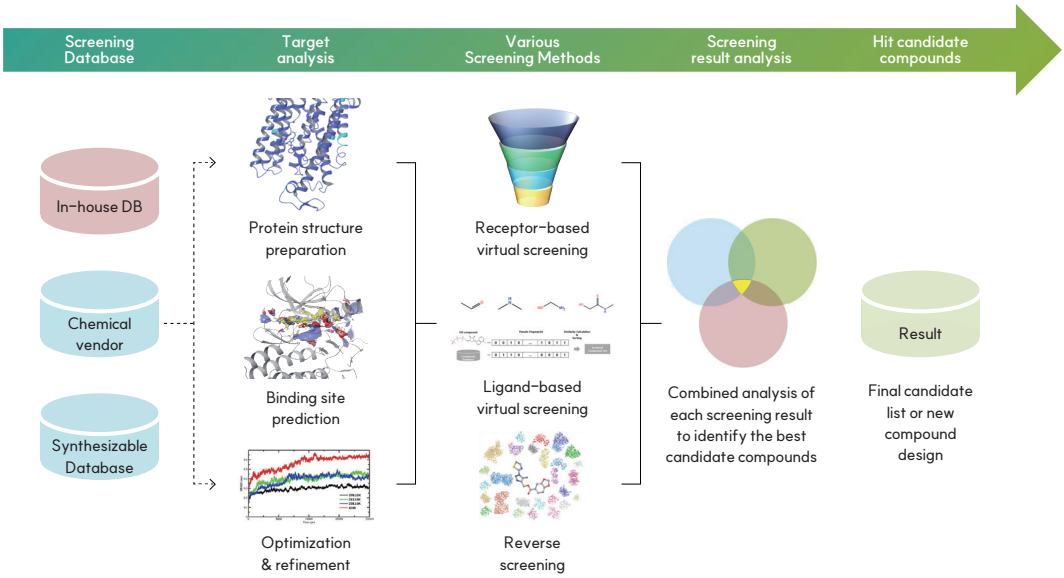
- Single analysis services
  (structural modeling, docking bond analysis)
- Research services
  (virtual screening, derivative design)

### ◎ Software Packages and Web Services

- Molecular modeling, AI data analysis package
- Development packages by field
  (small molecules, proteins, natural products)
- Characterization packages (toxicity prediction, PROTAC, PPD)

### ◎ Database Provision

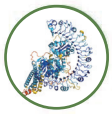
- Virtual screening, natural products, and protein structure libraries



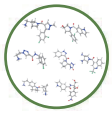

- Accurately analyze target protein structures and apply a range of screening assays
- Integrate data from multiple assays to identify the most promising candidate compounds

# *in silico* CRO Service

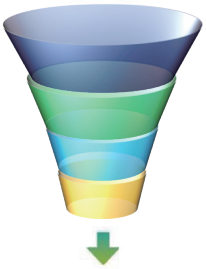
## Virtual screening service



• Target proteins



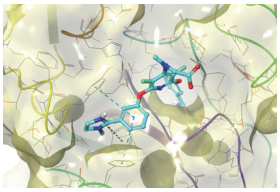
• Virtual Screening Library

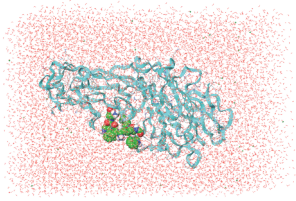


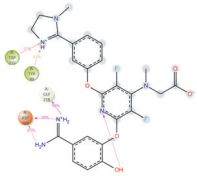
• Hit candidates

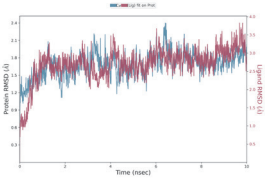
- Docking scoreguided selection
- Synthetic accessibility
- IP circumvention strategy
- Optimize the Synthetic scalability of the compounds
- AI-based ADME/T Prediction

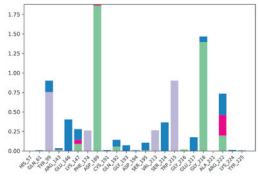
## Molecular docking and dynamics simulation



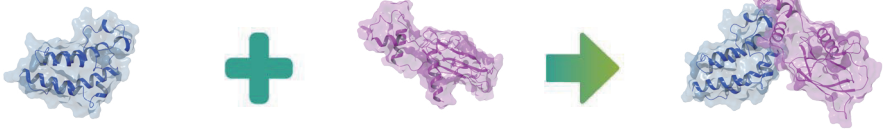






## Protein-protein docking



Protein A

Protein B

Complex A-B

## List of Available Services

### Target Validation

- Protein structure modeling
- Binding site analysis
- Molecular docking
- Molecular dynamics simulation
- Protein-Protein docking
- Reverse docking

### Hit Identification

- Receptor based virtual screening
- Ligand-based virtual screening
- Hyperscale virtual screening
- Shape screening
- Pharmacophore modeling
- Peptide modeling

### Hit to lead

- De novo design (AI)
- R-group Enumeration
- Scaffold-hopping
- Physicochemical property prediction
- ADMET prediction by AI

### Lead Optimization

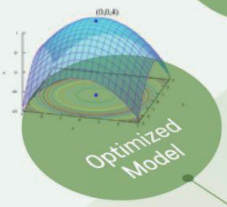
- Structure-based selectivity analysis
- Optimized structure design
- ADMET prediction
- Antibody maturation
- Protein engineering

# LNP AI Smart bench

## LNP Smart bench

Customizable cloud platform enabling digital transformation in drug discovery

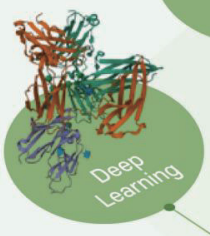

**User-friendly interface**
One-stop decision-making tool




**Optimized integration platform**
Leverage in-house data
World-class level of reliability


Enamine MolPort ChEMBL Tox21

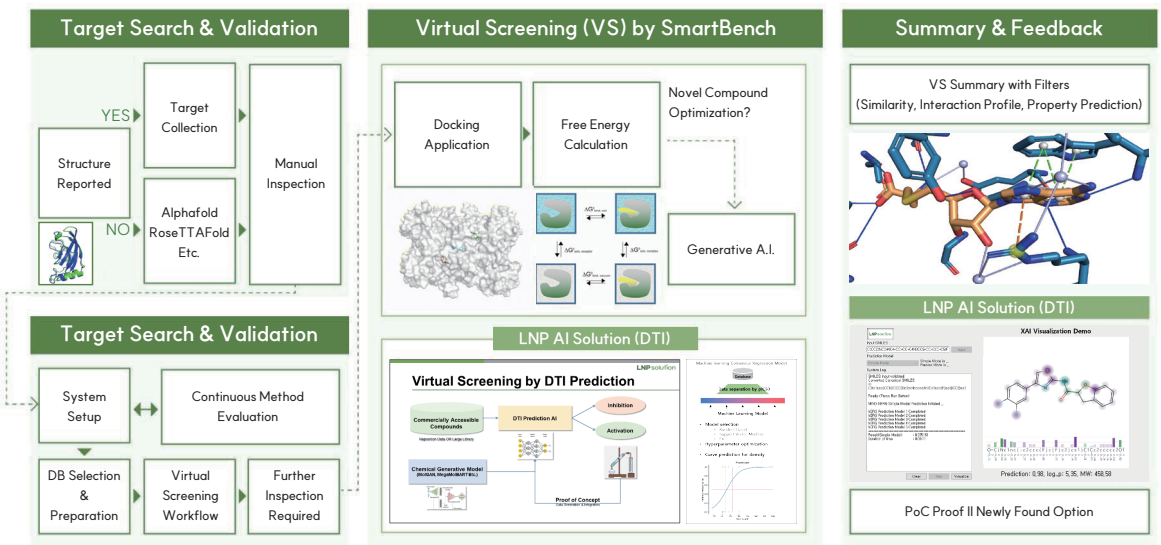
**Ultra-large compound library**
Over 30 billion compounds
Fast filtering system powered by deep learning




PyTorch docker DVC

**AI-powered open-source libraries**
The synergy of molecular modeling and deep learning
Extensive feature support

## Drug discovery workflow




## Cloud server system (Amazon, Nvidia GPU)

- Build a cloud-based platform without the need for on-premise server equipment
- Leverage the high security and reliability of cloud systems from Google, Amazon, and NVIDIA
- Enjoy ease of use through a user-friendly interface and intuitive settings

User-friendly cloud platform for intelligent, automated drug discovery

# Schrödinger Life Science Software

- Molecular modeling + AI software for small molecule drug discovery and biologics research
- Official partner for Schördinger Korea, the global leader in molecular modeling software, providing sales, support, and training for universities and government research institutes
- Distributed to government research institutes, and University
- Trial licenses and introductory training available
- Expert technical support and training for Schrödinger Software
- Various discount promotions and regular training sessions offered through our Korean office partnerships

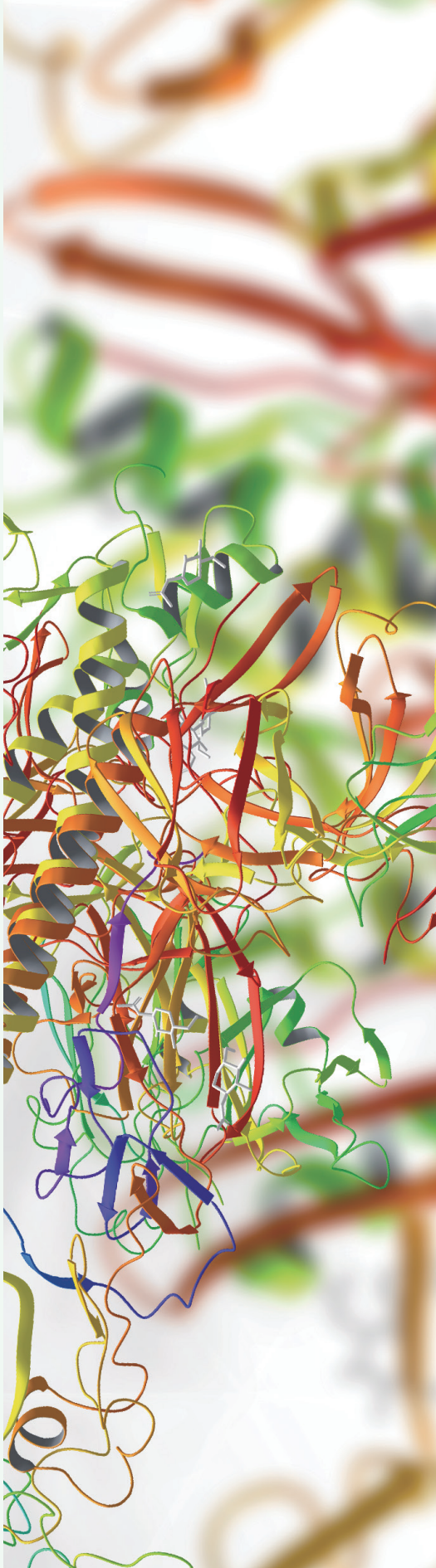
## Small molecule drug discovery

- Various virtual screening
- Shape-based screening
- Ligand-based pharmacophore modeling
- Lead optimization
- Deep learning for QSAR
- Refinement of protein crystal structures
- Structure analysis and homology modeling

## Biologics by design

- Antibody Modeling
- Reliable structure prediction from sequences
- Liability Prediction
- Rapid protein surface analysis
- QSAR analysis for biologics
- Applicable to antibody and standard (protein or nucleic acid) structures

Schrödinger



# Partnership

## Universities

고려대학교 KOREA UNIVERSITY

서울대학교 SEOUL NATIONAL UNIVERSITY

연세대학교 YONSEI UNIVERSITY

이화여자대학교 EWHA WOMANS UNIVERSITY

KNU 강원대학교

가천대학교 Gachon University

전남대학교 CHONNAM NATIONAL UNIVERSITY

조선대학교 CHOSUN UNIVERSITY

## Enterprises

medi 메디켐 chem

Global Leader of Cancer Treatments AUTOTELIC BIO 오토텔릭바이오

eFlask Collaboration, Development

국제약품 KUKJE PHARMA

kine sciences

ProviBio

OZ | ONCOZEN BIOTECH

Schrödinger

## Organizations

KIST 한국과학기술연구원 Korea Institute of Science and Technology

KRICT 한국화학연구원

Korea Chemical Bank 한국화합물은행

강원특별자치도 GANGWON STATE

재단법인 강원테크노파크 GANGWON TECHNOPARK

SKAI 스크립스코리아 항체연구원

강원지역혁신플랫폼 Gangwon Regional Innovation Platform

국립암센터 NATIONAL CANCER CENTER

K BIOHEALTH 오송첨단의료산업진흥재단

LNP Solution

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