DDC Service

DeepMatcher (Preclinical) Drug Candidate Service In 2 Years

syntekabio.com

Syntekabio

AI Drug Platform as a Service

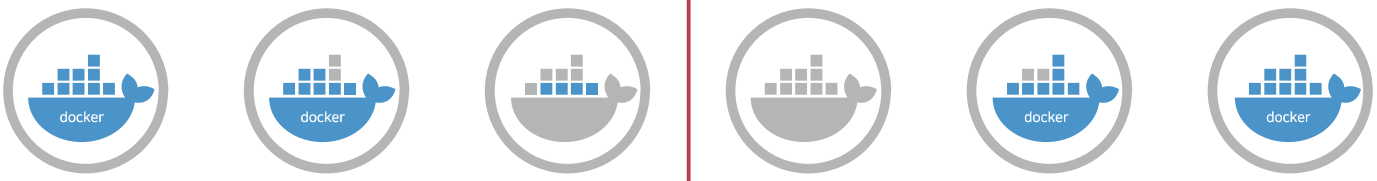
DDC STORY

- AI-driven DeepMatcher (Preclinical) Drug Candidate Service
- HIT to Preclinical Candidate in 2 YEARS
- Seeking Ultimate Success
- Service Process
- Cost Breakdown

DDC *AI-driven DeepMatcher (Preclinical) Drug Candidate Service*

DDC : HIT to Preclinical Candidate in 2 YEARS

HIT > LEAD > Candidate > Preclinical > Clinical > Precision Medicine



Hit Screening
DeepMatcher®-Hit

Lead Generation
DeepMatcher®-Lead

ADMET / PK
DeepMatcher®-ADMET / PK

GLP-Tox
FDA Registered Facility (CRO)

PGx Biomarkers for Drug Labeling
- Immunogenic Neoantigen Prediction
- Cancer/CNS Patient Stratification SNPs
- CYP typing, HLA typing & KIR typing

The Diagram shows Docker's extension to Syntekabio's AI-powered full drug discovery service solution that support almost all areas of drug discovery & development process from Hit discovery / Lead generation, and ADMET/PK to the pharmacogenomics biomarkers. It is based on Syntekabio's powerful AI technologies (DeepMatcher®) that provide the best docking Hits/Leads through analysis of deep learning (3D-CNN) and MD simulation on targets. Docker is a virtualization software.

"UNMATCHED SUPERCOMPUTING TO SUPPORT YOUR DRUG-DISCOVERY & DEVELOPMENT PROJECTS"

A-Z Package

Hit-Discovery, Assay Validation, Lead Generation & Preclinical Study

Client-Centric

Minimal Risk * Maximum Customization

In-House & Global CRO Cooperation

Discovery & Development

Infra-structure

- **Fully Customized Packages & Services** to Ensure High Success Rate
- **Bio-Supercomputer** Capacity for Bio-Research, Medicine & Pharmacology

Experiences

- **15+ Years Experience** on Machine-Learning + Structural biology + Supercomputing
- **AI & GPT** Accelerates Screening Flows and Calculations and increase success rate
- **30+ Affiliations & Partnerships** with Certified Global CRO Expert Groups

Owner-finance

- **7.5% Down Payment of Total $cost** to Start & Installments for Pay As You Go Model
- **Flexible Timeline & Milestone** to Match Client's Finance & Convenience

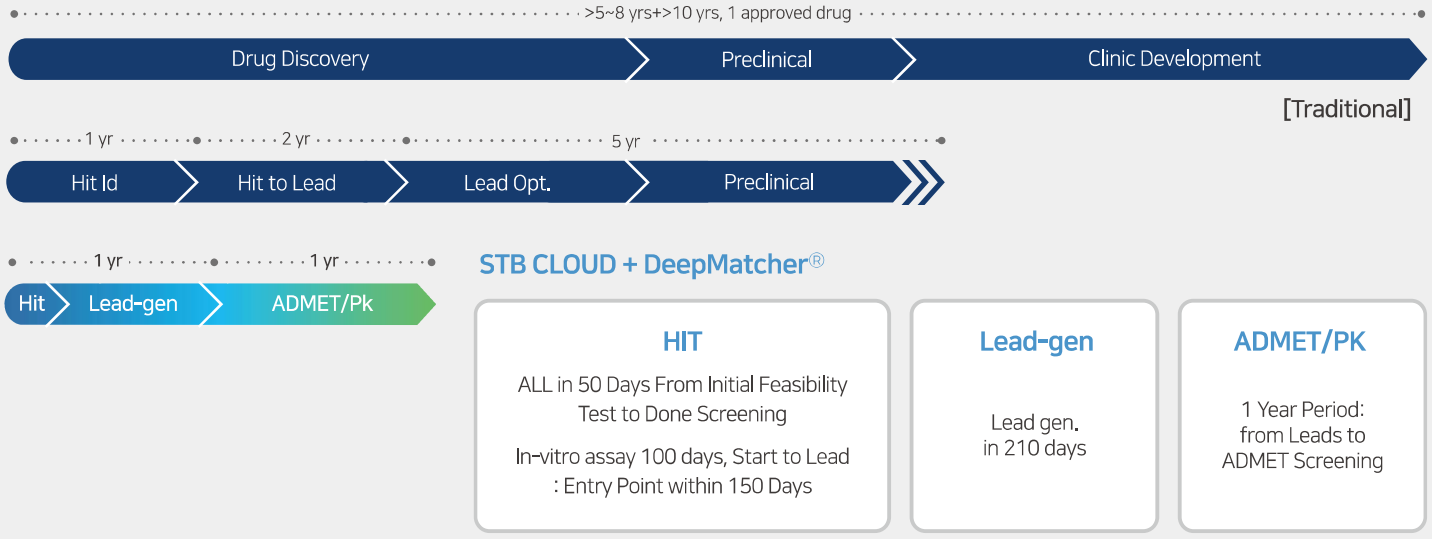
All in one

- From Start-to-Finish A-Z Services = **Identify Preclinical Drug Candidate in 2 YEARS & Support IND Preparation**

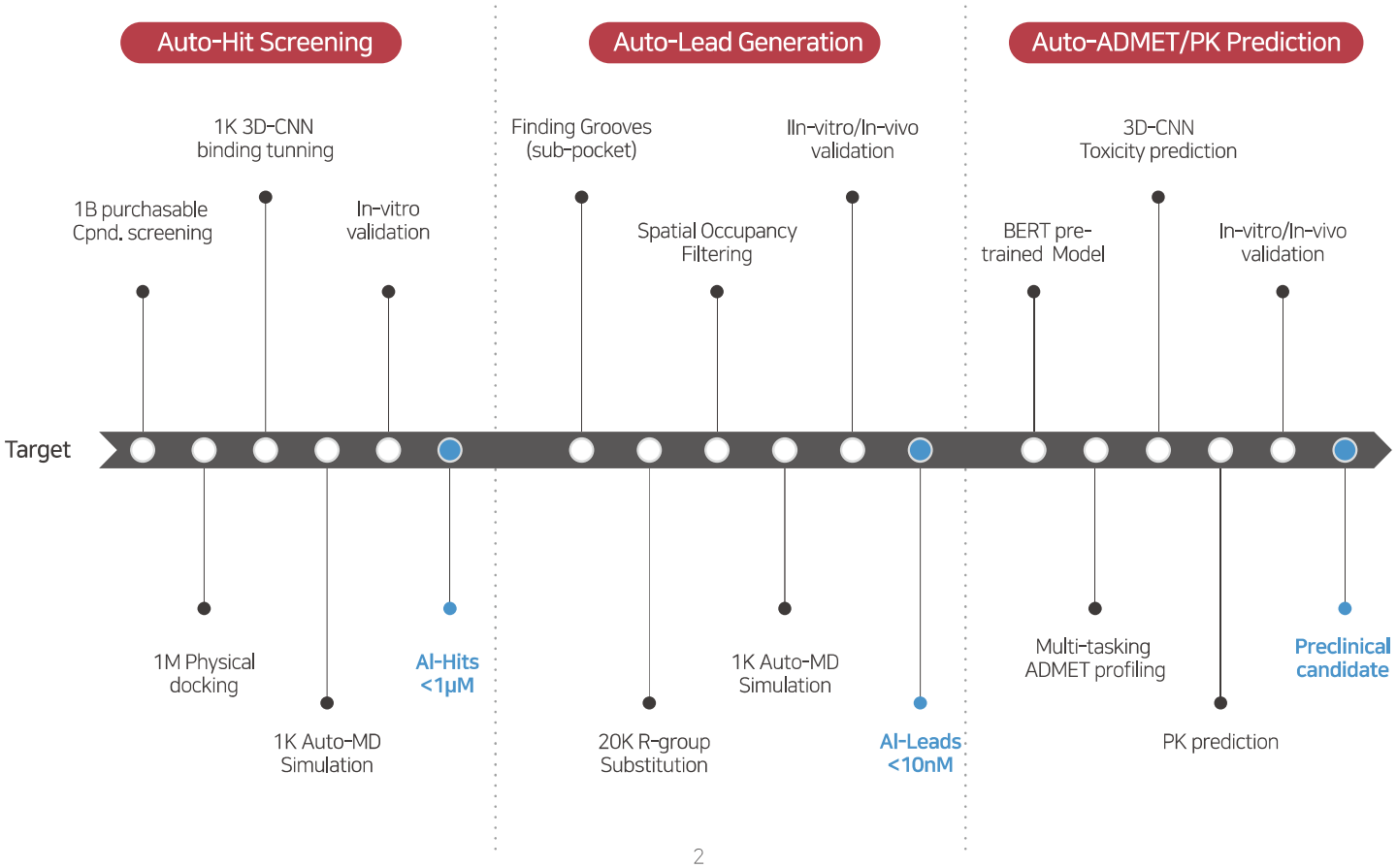
HIT to Preclinical Candidate in 2 YEARS

·AI Bio Supercom(ABS) Center with 10,000 servers (in progress)

·Cloud based AI Bio Supercom(ABS) Center serves best-in-class solutions for AI drug discovery



DeepMatcher (Preclinical) Drug Candidate : DDC framework



Seeking Ultimate Success

·AI-powered auto-HIT/Lead discovery: DDC, as a successful loop platform

1 Auto-Hit Screening

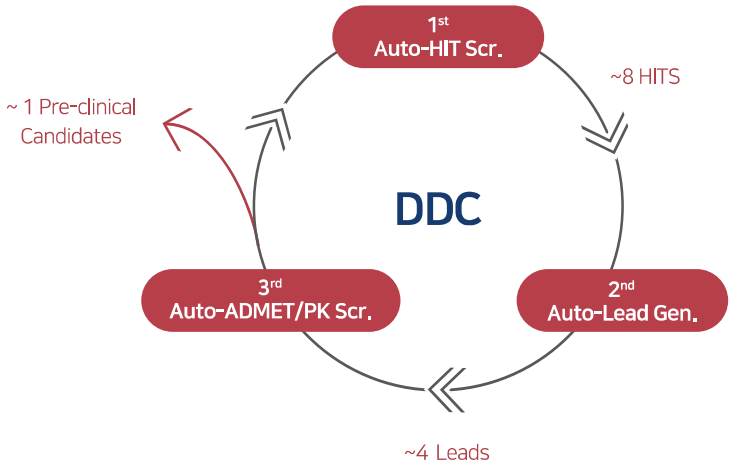
Purchasable 1B Chemical Library Screening
Physical-3D Docking (1M)
3D-CNN Pose Tunning (1K)
Auto-MD Simulation Fine Tunning (1K)

2 Auto-Lead Generation

Sub-pocket & Week bond Screening
Substitution of 20K R-group to Scaffold
Free Energy Perturbation in the Sub-pocket
Auto-MD Simulation Fine Tunning (1K)

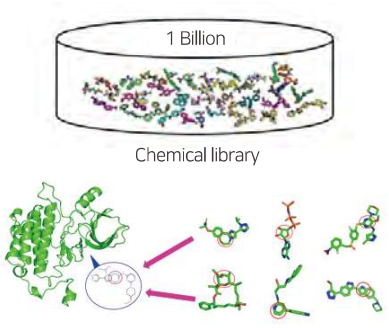
3 Auto-ADMET/PK

Solubility, Intestinal Absorption, Metabolism, PPB, BBB
Liver injury, Off target toxicity (NR, HLA adduct, Signaling), PK, etc.

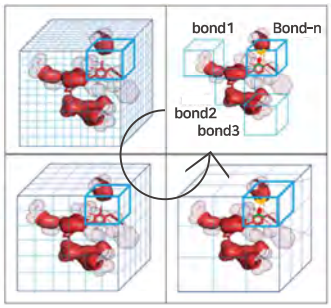


·Deep Learning: Strength in docking & best pose generation similar to real 3D structure
·Auto-MD simulation: Strength in binding energy calculations close to experimental values
·GPT: Strength in virtual screening by cognitive learning based on big data and extreme hardware

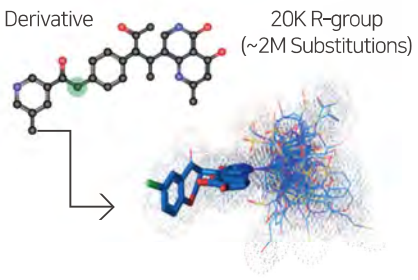
Chemical Library screening



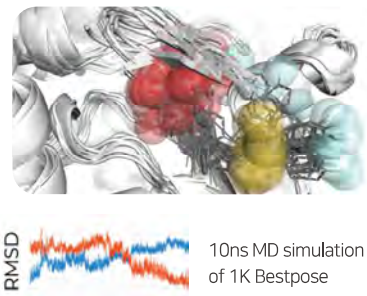
3D-CNN Binding Tuning



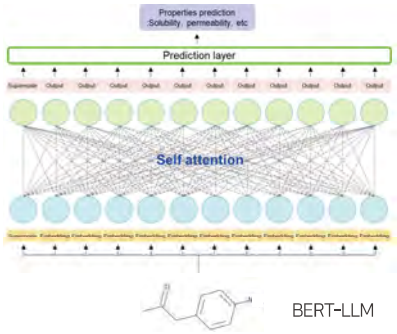
R-group substitution



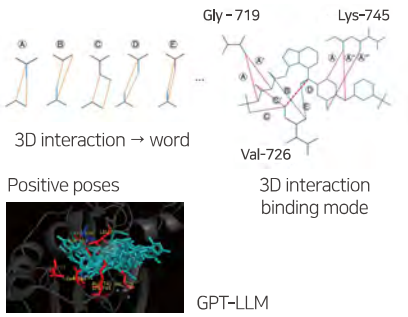
Auto-MD Simulation



BERT - ADMET/PK screening



3bmGPT - key residue analysis



Service Process

Step	Items	Core Technology	TPP	Duration
Hit Discovery	AI-HIT discovery	[1]DMC-Hit®	IC50 < 1μM ~8 Hits	~ 2 m
	AI-Hit purchase			~ 3 m
	Hit confirm			
Lead Generation	AI-LEAD generation	DMC-Lead®	IC50 < 10nM ~4 Leads	~ 7m
	Compound synthesis & Lead confirm			
	Go-No Go Decision (1st Year)			
ADMET/PK (Preclinical Candidate)	AI-ADMET generation	DMC-ADMET/ PK predictor®	Decent ADMET /PK Profiles ~1 Candidate	~ 12 m
	Compound synthesis			
	ADMET validation			
	PK validation in mice (PO)			
	Success-Failure Decision (2nd year)			

[1]DMC: DeepMatcher

Cost Breakdown

Unit	Hit Discovery	Lead Generation	ADMET/PK	Total
Hardware/computation (single service only*)	1000 Servers /1~2 Month	1000 Servers /1~2 Month	1000Servers /1~2 Month	
	$150K	$150K	$150K	
Chemical Purchase/Synthesis/Assay (Validation size)	~200 chemicals	~ 40 Chemicals	~ 20 Chemicals	
	$20K ($100/purchase)	$293K (10mg/synthesis)	$200K (~150mg/synthesis)	
	$30K ($150/assay)	$7K ($150/assay)	$400K ($20K/assay)	
Estimated Cost sum	$200K	$450K	$750K	$1.4 Million
BigPharma Traditional R&D Cost[4]	$1.0M	$12.5M		$13.5M

Medium.com/EvinceBio, 2017 report

References:
1. Syntekabio's Hit to Preclinical Candidate on Cloud Computing, **BioPharmaTrend**, Vol4. 2023
2. How Syntekabio's Supercomputing Enables AI-driven Drug Discovery, **BioPharmaTrend**, Vol3. 2023
3. The Power of STB CLOUD in Remote AI Drug Discovery, **BioPharmaTrend**, Vol2. 2023
4. The State of A.I. Drug Discovery and Its Future: Small Molecules, Vaccines, and Antibodies, **BioPharmaTrend**, Vol1. 2023

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