

DR.NOAH BIOTECH Inc.

[NeuroRG[®]] Deep Learning Based High-Throughput Screening Platform



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- IV** 공모전 Q & A

I. INTRODUCTION



| CEO: Dr. JIHYUN LEE



- CEO, Founder, DR.NOAH BIOTECH (2017.01 – Present)
- Research Professor, BioCon & Seoul National University (2016 – 2018)
- Ph.D. in Pharmacy, Seoul National University (2013)
- MSc in Computing, Manchester Metropolitan University (2007)
- BSc in Biological and Computing Science, The University of Manchester (2006)

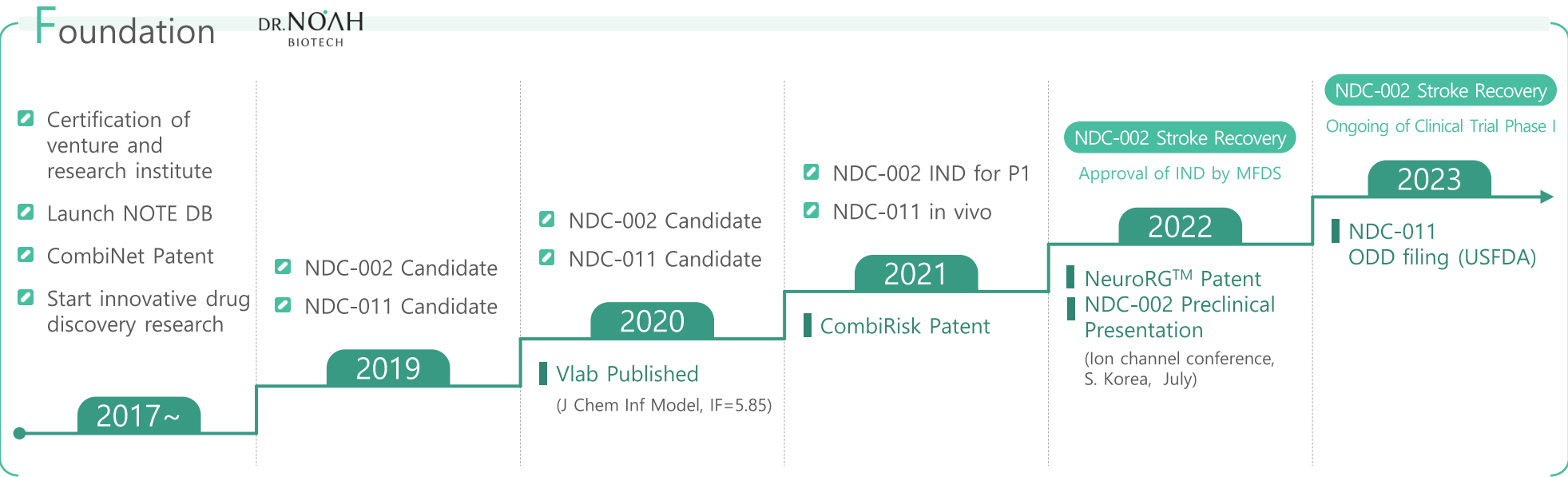


| Mission

Development of **New Combination DRUGs**
based on **Bio-pharmacological Big Data Analysis**
and **Artificial Intelligence Technology**

| Vision

For **PATIENTS** somewhere in the world,
let's make a **New Combination DRUGs**
that's not anywhere else in the world



Individuality

Innovative AI technology to essential for the pharmaceutical industry (Combination drug)

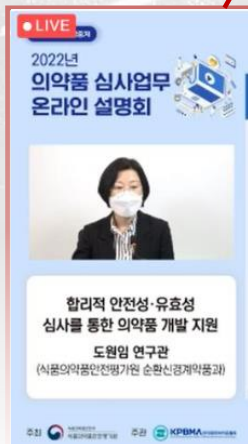
Commercialization

Quickly commercialize new drugs.

Scalability

AI platform that can be expanded to healthcare.

Korea FDA established the screening criteria for new drug candidates derived by AI



미래를 향한 의료 미래를 여는 뉴스
MEDI:GATE NEWS
기사입력시간 22.04.14 06:57 | 최종 업데이트 22.04.14 06:57
AI로 도출한 신약 후보물질은 어떤 기준으로 심사할까?

뿐만 아니라 인공지능(AI)으로 신약 후보물질을 도출하는 기업들이 많아지면서, 이에 대한 심사 기본 원칙과 방향도 수립했다.

한편 식약처는 의약품 안전 정보와 정확한 임상시험 정보 제공을 보다 강화하기 위해 전문가용 임상시험 정보 작성 가이드라인도 마련한다. 임상시험 정보 기재에 포함되는 임상시험 여부와 개개 시험을 설명하는 방법, 시험 결과를 제시하는 방법 등을 담은 예정이며, 오는 6월에 마련·배포할 계획이다.

닥터노아바이오텍, 뇌졸중 치료제 국내 1상 승인

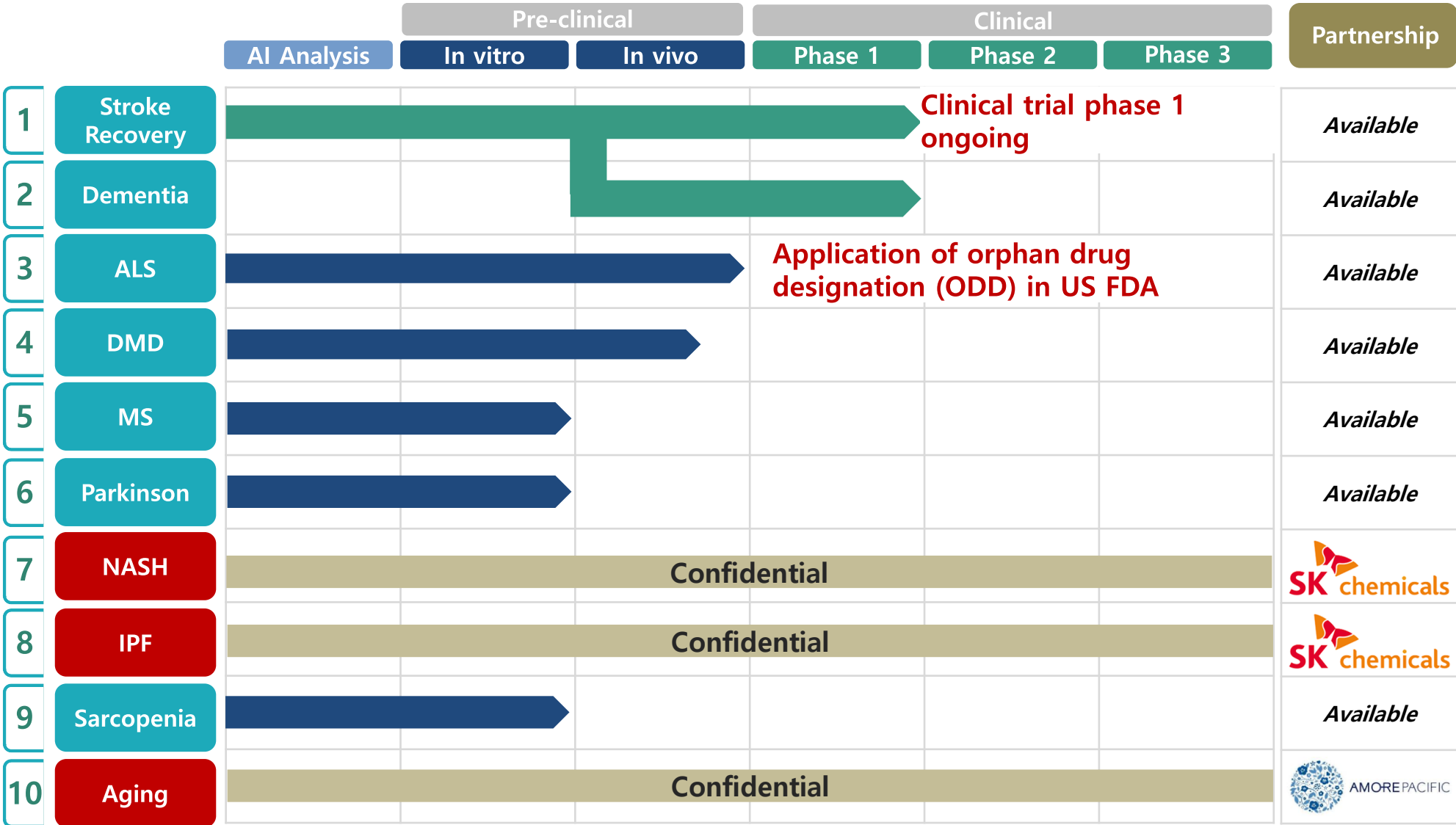
AI 플랫폼 기반 발굴·이중기전 후보물질 본임상 첫 승인 사례

최은수 기자 | 공개 2022-04-22 08:37:00



DR.NOAH BIOTECH,
Approved clinical trial phase 1
for stroke recovery in South Korea

NEW COMBINATION DRUG PIPELINE

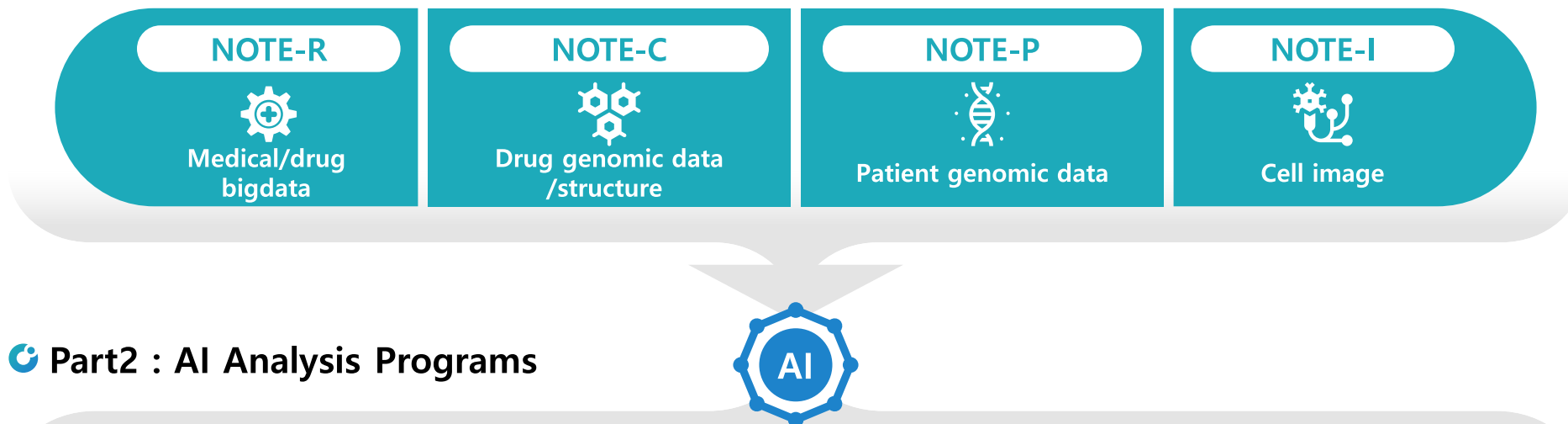


Abbreviations **ALS** = Amyotrophic lateral sclerosis, **DMD** =Duchenne muscular dystrophy, **MS** = Multiple Sclerosis
NASH = Non-alcoholic Steatohepatitis, **IPF** = Idiopathic Pulmonary Fibrosis

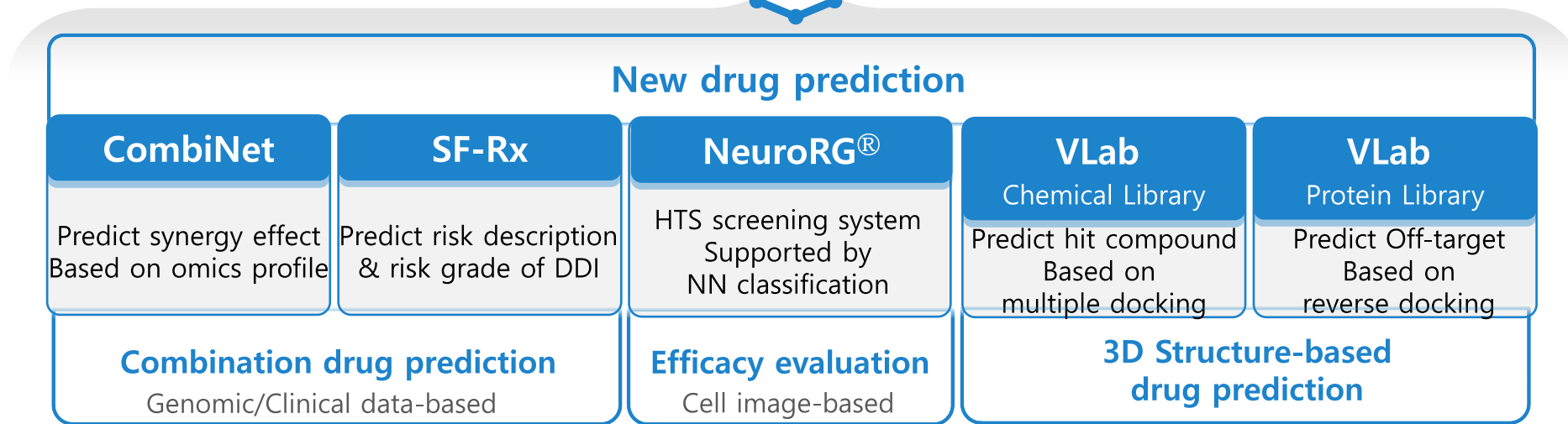
II. DR.NOAH BIOTECH's AI SOLUTION



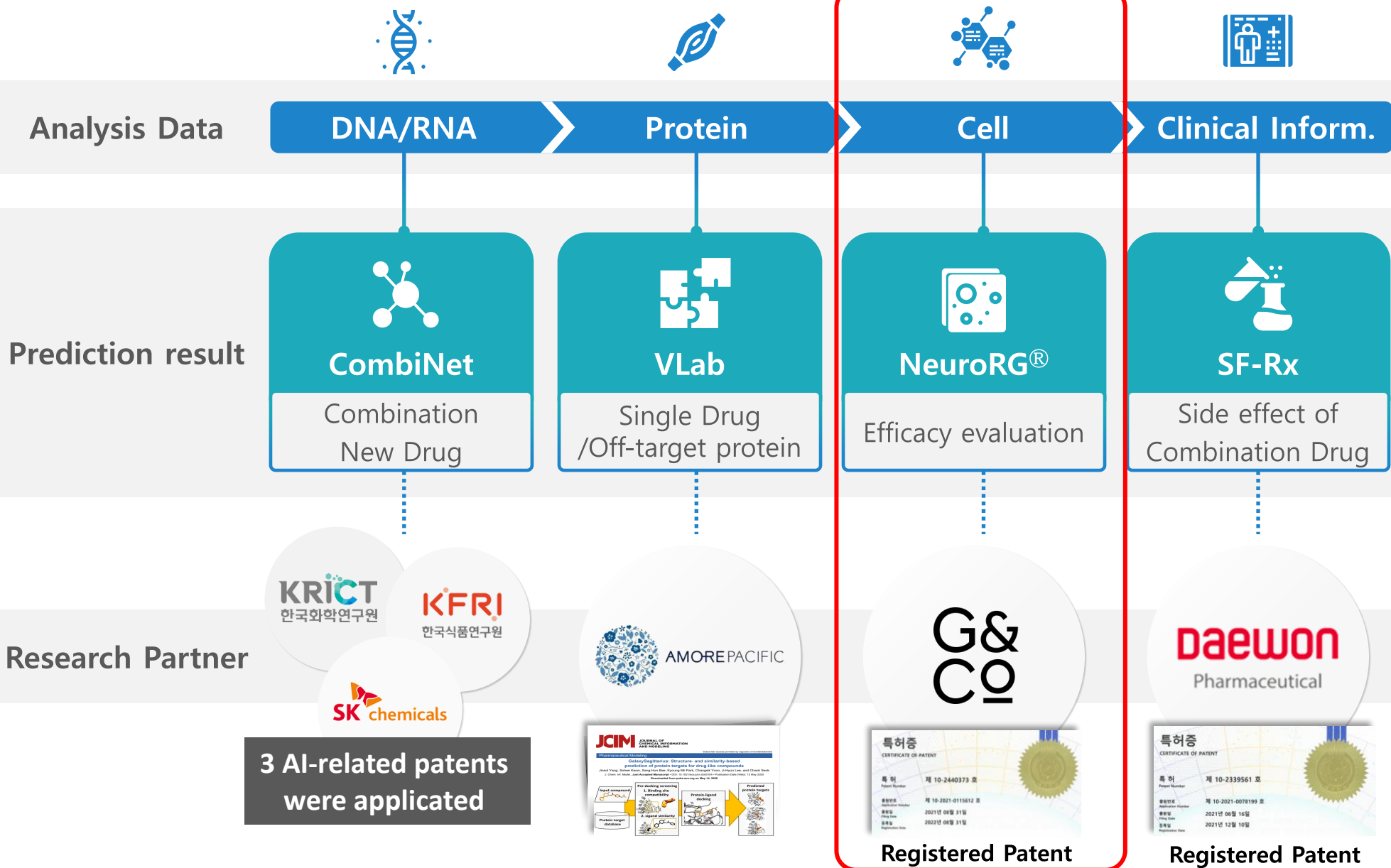
Part1 : NOTE Databases



Part2 : AI Analysis Programs



ARK: AI-BASED DRUG DESIGN PLATFORM



CombiNet – New combination drug prediction platform

1 Data preparation for prediction

NOTE-P



Patient
genomic data

NOTE-C



Drug
genomic data

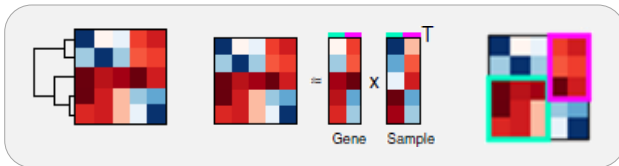
NOTE-R



Medical/drug
bigdata

2 Dynamic Module Detection

Clustering/Decomposition/Bi-Clustering



Diverse pathological networks

3 Network Evaluation



Network evaluation
with functional enrichment



Combination drugs
eliciting synergistic effects
on pathological networks

5 Prediction of synergistic drug pair

Pair #1



→ Synergistic

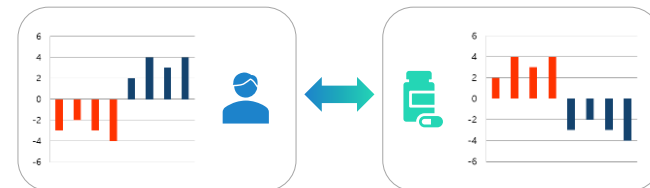
Pair #2



→ Antagonistic

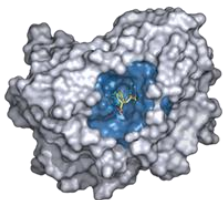
4 Drug prediction for networks

Comparison of patient and drug expression patterns



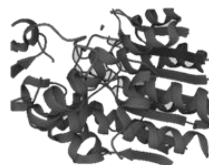
Vlab - 3D structure-based drug/protein prediction platform

Multi-docking Simulation



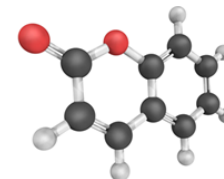
- 4 different types of binding scoring function & scores
- SCORE_RB_PEN
- SCORE_NORM_HEVATOMS
- SCORE_NORM_CRT_HEVATOMS
- SCORE_NORM_WEIGHT
- CHEMparthbondCHO

Protein binding site features



- Surface area
- Volume
- Amino acid composition
- Amino acid composition at the binding site surface
- Number of residues
- Composition of C, N, O, S atom Elements

Compound features



- Predicted logP
- Number of H-bond donors & acceptors
- Number of atoms
- Number of rotatable bonds
- Topological polar surface area
- Composition of atom elements (C, N, O, S, P, F, Cl, Br, I, H)

Deep learning
VLab

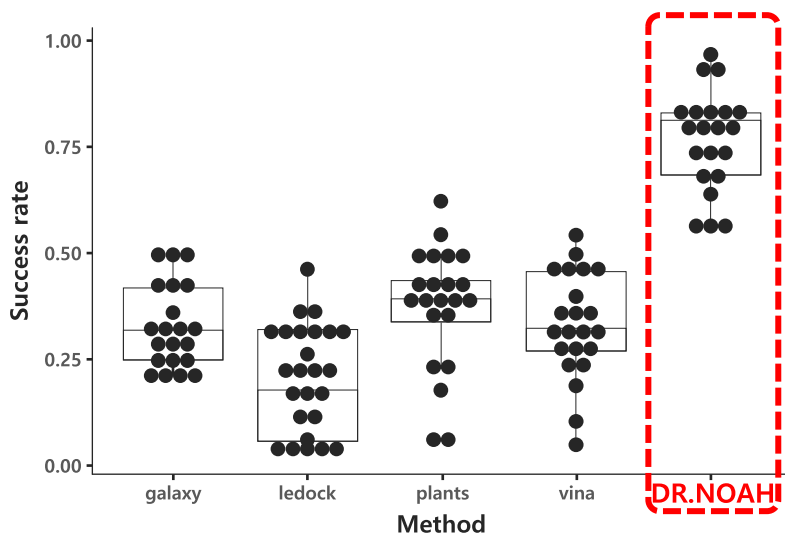


- Sophisticated calculation with Multi-docking simulation
- Both Docking/Reverse docking possible

- Docking: Searching compounds to bind to proteins
- Reverse docking: Searching off-target of compounds

Vlab - 3D structure-based drug/protein prediction platform

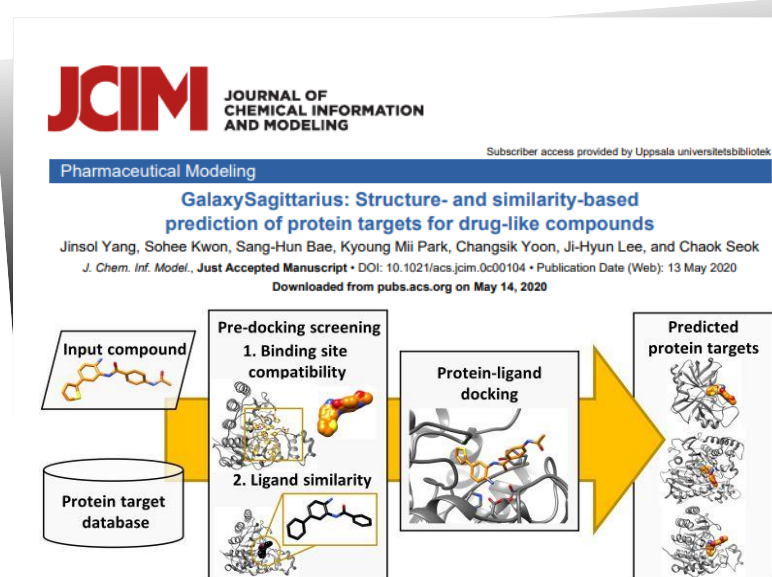
Evaluation of drug prediction performance



Success rate

- Check how many drugs are actually effective among the predicted drugs
- Existing software: 0.2 ~ 0.35
- DR.NOAH's software: 0.76
- Stable and high accuracy confirmation

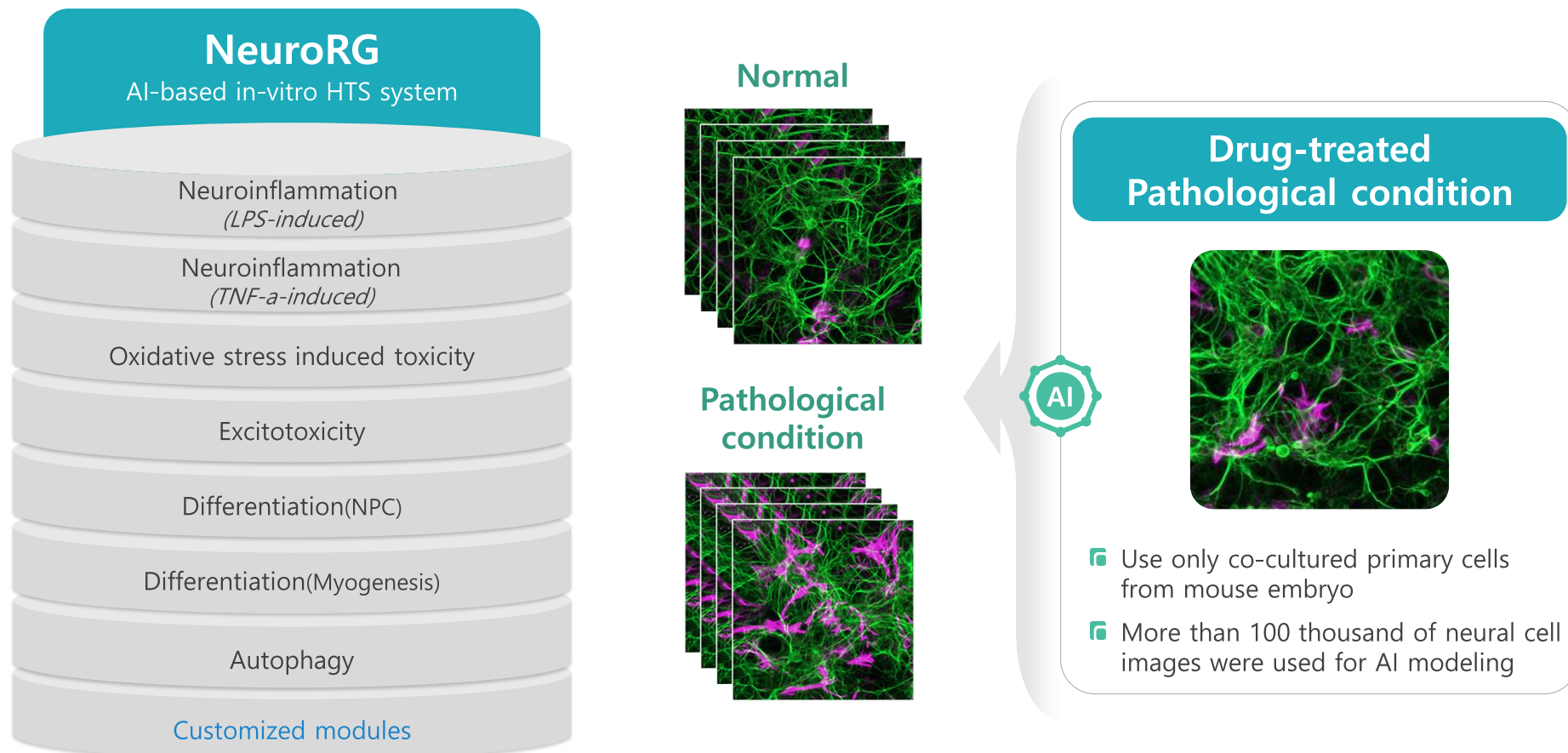
JCIM published in May 2020



AMOREPACIFIC

Revenue recognition

NeuroRG® - Deep Learning Based High-Throughput Screening Platform



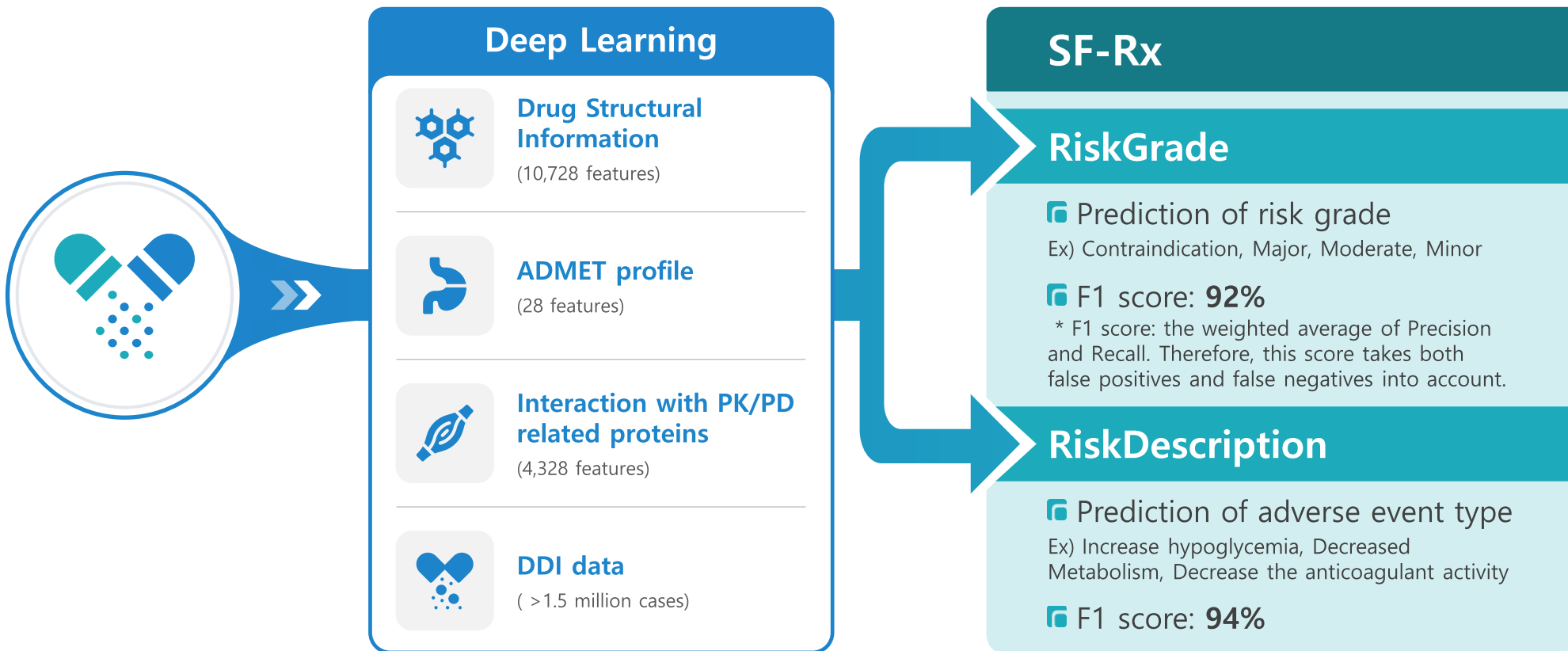
Production of images for accurate drug efficacy evaluation

1 year = 10 million (100 billion cells) image production



**Patent registered
in 2022**

SF-Rx – Risk of combination drug



**Major
Achievements
In 2021**

① Collaborative research with Global pharmaceutical companies in Korea

**Revenue
recognition**

(Clinical trial ongoing)

daewon
Pharmaceutical

② Patent registration (Dec. 2021)

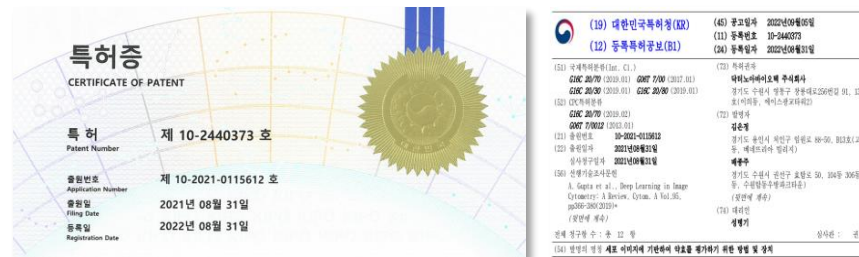


III. NeuroRG®

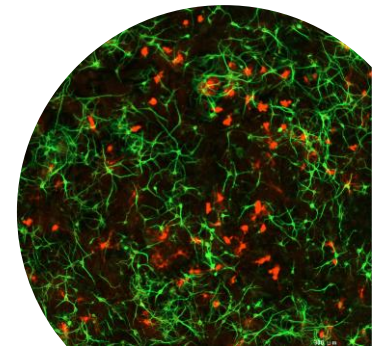


Overview

- **Efficacy evaluation with specific modules for each disease**
- Quick evaluation **with automated facilities in DR.NOAH BIOTECH's research center**
- Possible to complete **evaluation of 10,000 drugs within 2 months** (with HTS facility)
- Possible to evaluate with various cells (**primary cell**, cell line, iPSCs) and **co-culture cells**
- **Deep-learning based screening by visualization**
 - ✓ Cell's morphological change
 - ✓ Expression of target protein (e.g., GLP-1, PD-L1)
 - ✓ Specific biomarker (e.g., aging, differentiation, EMT, cell interaction, cell membrane)
- **Intellectual property** (Patent registered in South Korea)



Patent (10-2440373KR)



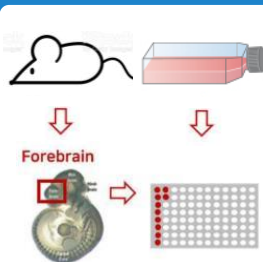
Research flow

Step 1 & 2

Modulization

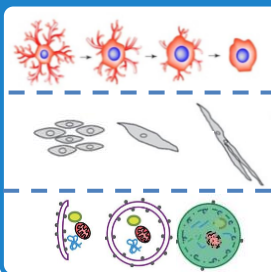
(Preparation & AI Training)

Preparation



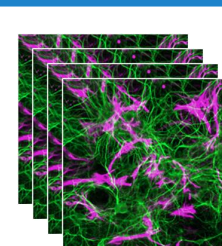
- Primary cell culture
- Cell line culture
- iPSC
- Etc.

Condition setup



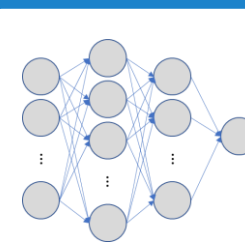
- Neuroinflammation
- Myogenesis
- Autophagy
- Customized set-up

Mass cell image generation



- 1 year = 10 Million images (100 billion cells)
- 1 day = 200GB (30 movies)

AI Training

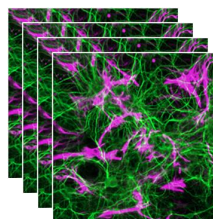


Drug Library

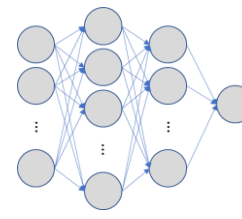


- Client's library
- DR.NOAH's library

Treatment



Efficacy prediction



Hit ranking

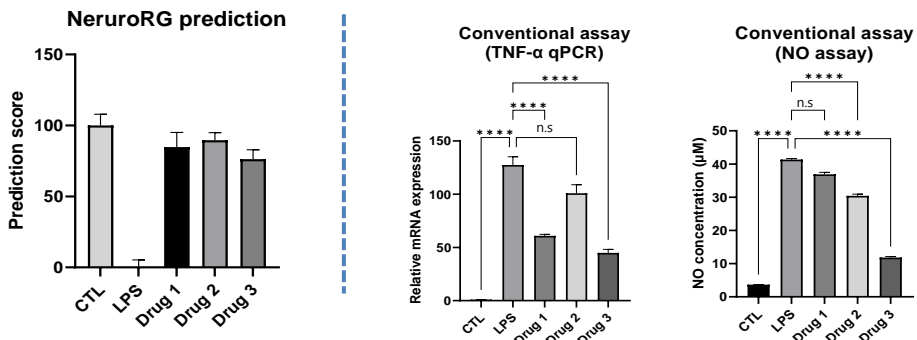
Rank	Drug	Hit Score
1		<div></div>
2		<div></div>
3		<div></div>
4		<div></div>
5		<div></div>

- **Option: identification of Hit compounds with bio-assay**

Example1: Neuroinflammation module

High Accuracy

94.4%

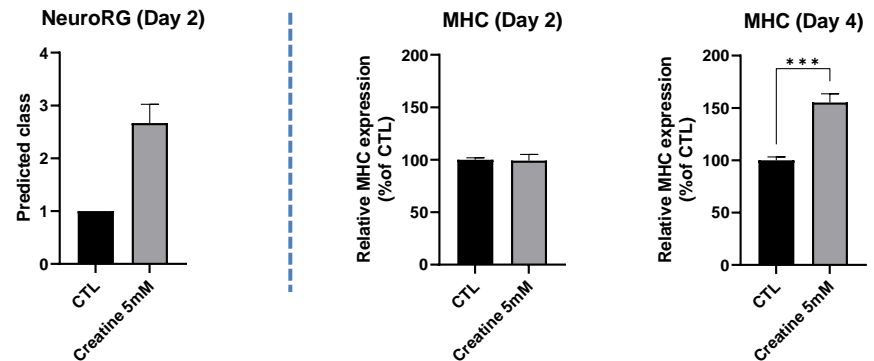


- NeuroRG[®] : 약물의 endpoint인 morphology를 감지하여 약효를 정확히 검출 (정확도 94.4%)
- 기존 방법 : assay의 종류에 따라 후보물질간 결과 차이가 있음 (Drug 1은 TNF-a실험에서는 효과가 있지만, NO실험에서는 효과가 없음)

Example2: Myogenesis module

Reduced Time




1/6배



- 1천개 화합물 스크리닝 소요 시간 비교 (실험자 1명, 반복횟수 3회, 농도 3종류 기준)

NeuroRG [®]	Conventional assay (MHC assay)
5 weeks	28 weeks

NEURORG® TECHNOLOGY – APPLICATION

		Pre-clinical		Clinical			Partnership	
		AI Analysis	In vitro	In vivo	Phase 1	Phase 2	Phase 3	
1	Stroke Recovery	COMBINET	Clinical trial phase 1 ongoing				Available	
2	Dementia						Available	
3	ALS	COMBINET	Application of orphan drug designation (ODD) in US FDA				Available	
4	DMD	COMBINET					Available	
5	MS	COMBINET					Available	
6	Parkinson	COMBINET					Available	
7	NASH	COMBINET	Confidential					
8	IPF	COMBINET	Confidential					
9	Sarcopenia	NEURORG®					Available	
10	Aging	COMBINET	Confidential					

Abbreviations

ALS = Amyotrophic lateral sclerosis, DMD =Duchenne muscular dystrophy, MS = Multiple Sclerosis
 NASH = Non-alcoholic Steatohepatitis, IPF = Idiopathic Pulmonary Fibrosis

Best Solutions to Speed-Up Your Drug Discovery



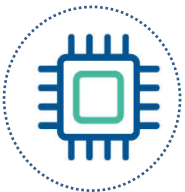
High speed, high accuracy and less cost



Efficacy evaluation with specific modules



Evaluation of various cells and co-culture cells



Deep-learning based high-throughput screening

IV. 공모전 Q&A



Q1 서비스를 무료로 제공하는 목적은? & 선발 기준은?

- **NeuroRG®의 성공사례 창출/ 고객사의 니즈 충족**
 - ✓ 고객사에서 자체 보유중인 라이브러리 중 신규 유효물질을 발굴
 - ✓ 자체 보유 약물과 FDA승인약물 (닥터노아바이오텍(주) 제공 예정)과의 병용 효력 발굴
- **선발기준**
 - ✓ NeuroRG 활용 목적이 뚜렷하고, 결과가 고객사의 연구개발에 핵심적인 요소가 될 경우

Q2 전통적 방법과의 차이점은?

- **소요시간 감소 & 높은 정확도**
 - ✓ ex. 근육세포 분화 실험: NeuroRG® (5주), 기존 assay (28주) → **약 6배의 시간 감축 효과** (약물 1천 개, 3 반복 실험 기준).
 - ✓ ex. 신경세포내 항염증물질 발굴: co-culture에서 microglia의 표현형의 변화를 AI가 정확하게 판단하여 유효 물질을 발굴 (정확도 94.4%)

Q3 고객사에서 제공하여야 할 정보는?

- **공모전 신청서 [양식1]를 작성하여 지원**
 - ✓ 최종 선별된 고객사: 자체 보유중인 약물 라이브러리, 실험에 활용되는 세포 제공
 - ✓ 일부 FDA승인 약물 (300여종)은 닥터노아바이오텍(주)에서 제공 가능

Q4 비밀유지 및 의무 사항은?

- **비밀유지계약 및 서비스 계약 필수**
 - ✓ 최종 선별된 고객사: 향후 닥터노아바이오텍(주)의 플랫폼 홍보 활동에 협조 (비밀유지계약내 포함.)

Q5 성과물에 대한 IP (지식재산권, 특허)는?

- **100% 고객사 소유 (비밀유지계약 및 서비스 계약내 포함.)**
 - ✓ 중간 또는 최종 결과물에 관한 소유권 및 지식재산권법 상 권리는 100% 고객사 소유
 - ✓ 단, 서비스 범위 외에 소요되는 연구 또는 실험에 대해서는 상호협의 하에 결정

Q6 기타 문의 사항

- **bsd@drnoahbiotech.com로 문의**

Thank You

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