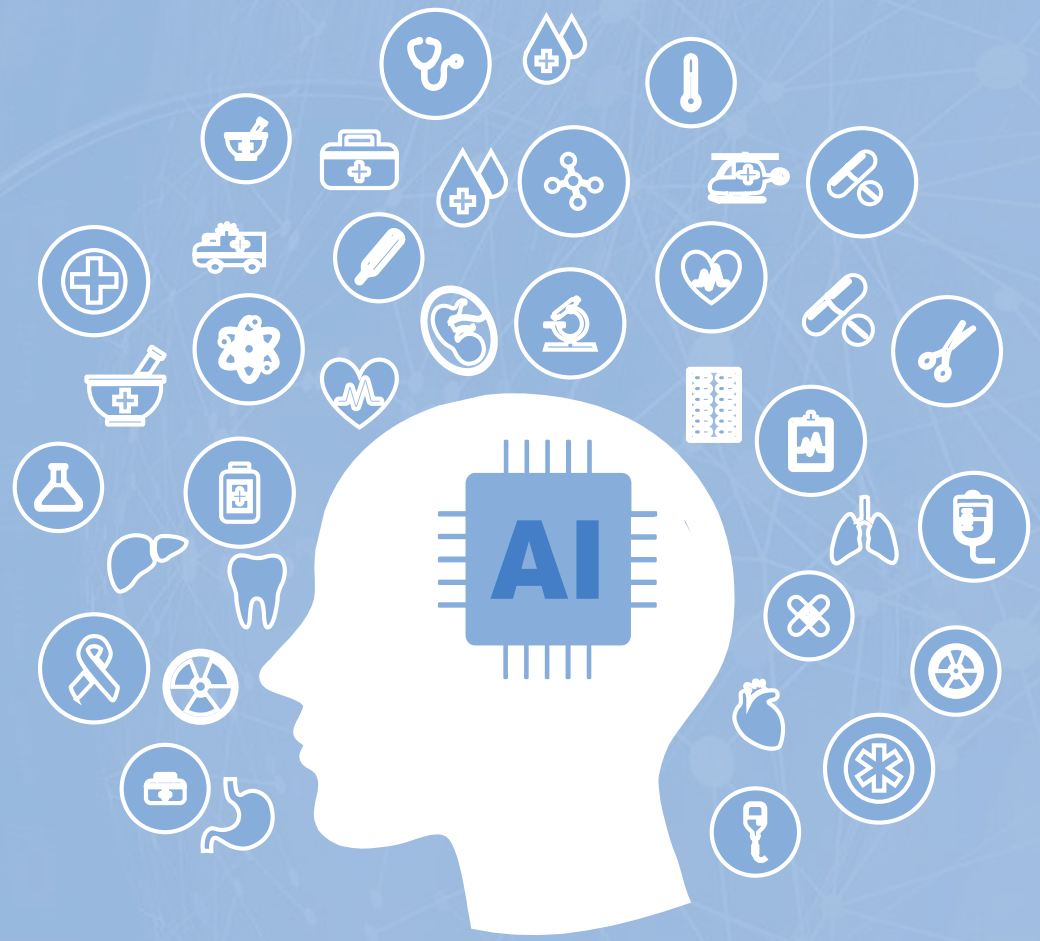
AIGENDRUG
artificial intelligence for drug discovery

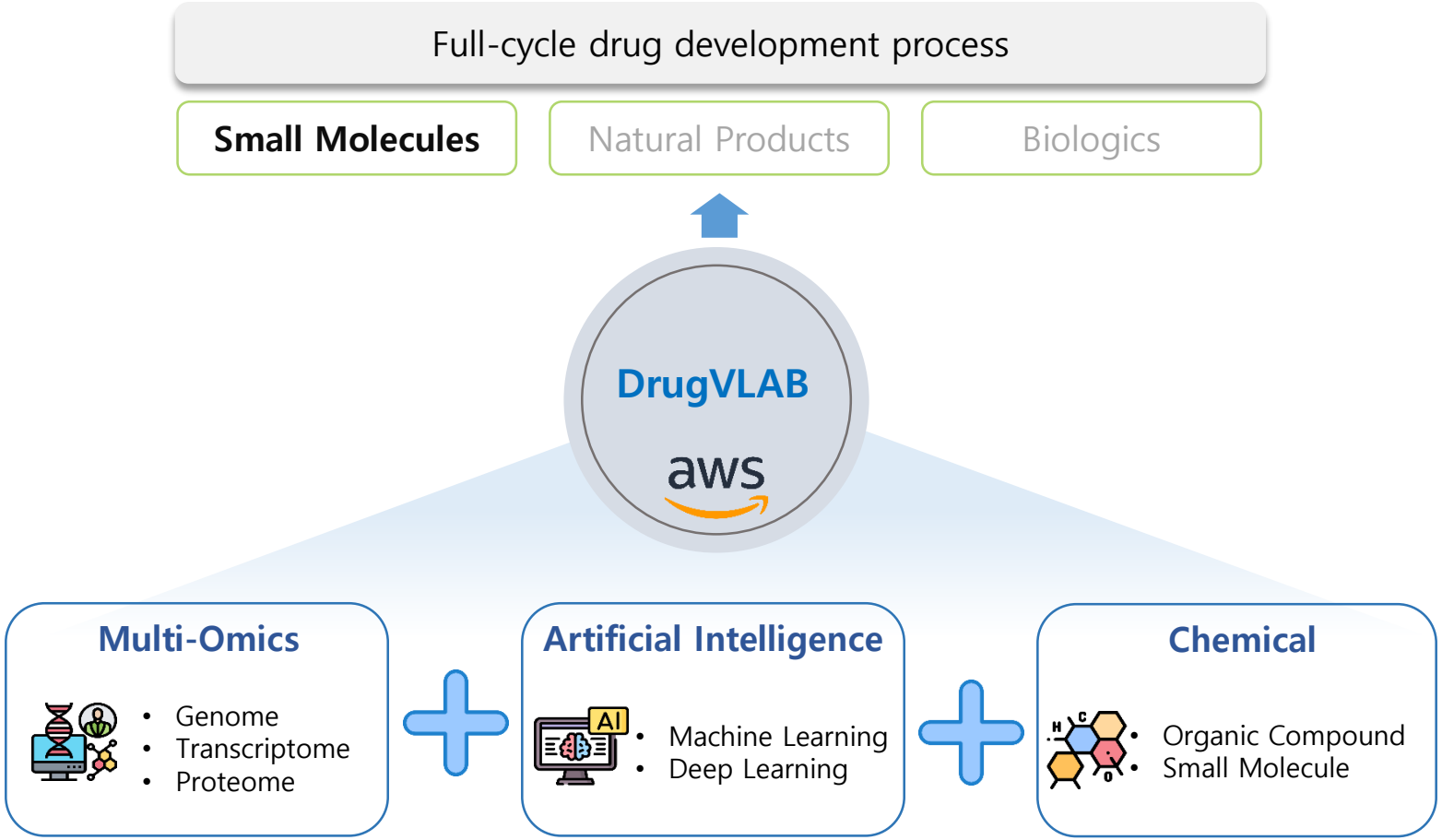


인공지능 신약개발 플랫폼 기업

AIGENDRUG Co., Ltd.

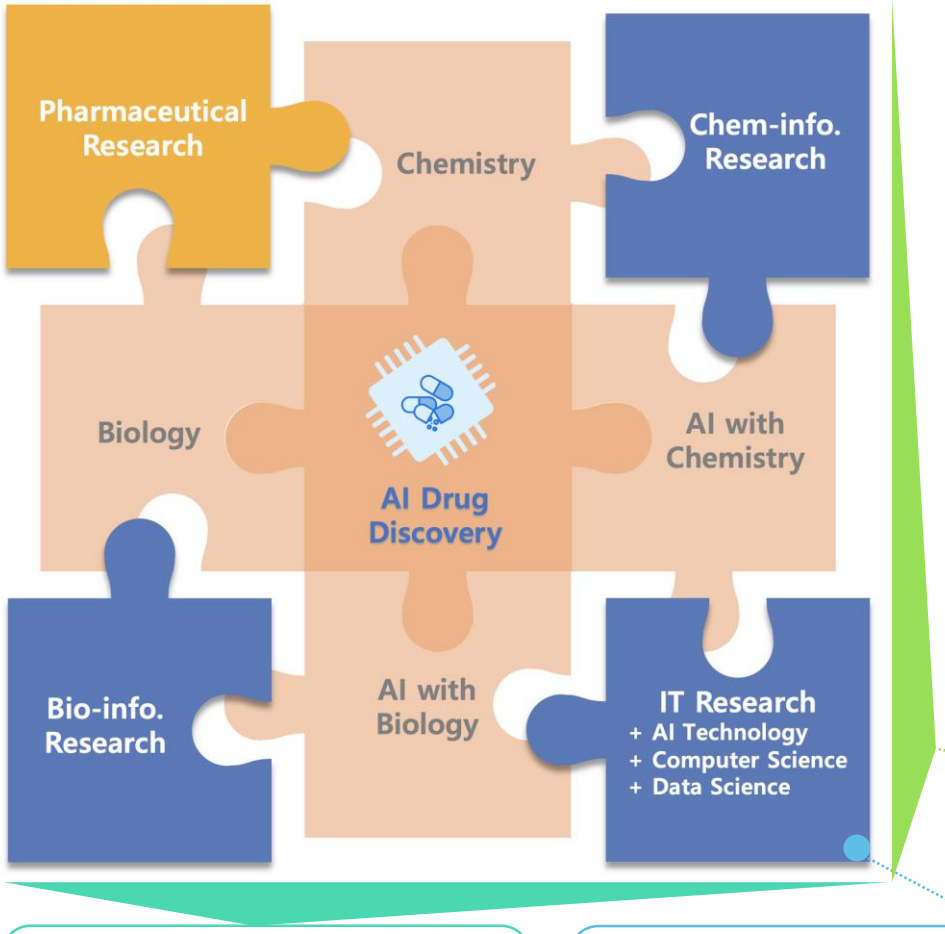
AIGENDRUG
artificial intelligence for drug discovery

Contributing to **Human Health** by **Broadening Drug Research**

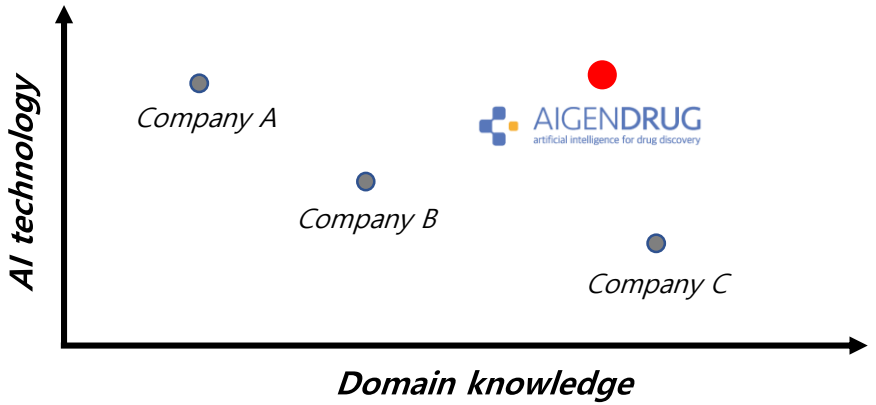


02 Competitiveness

AIGENDRUG
artificial intelligence for drug discovery



"Fully customized AI service tailored specifically for your needs"



- **150+ SCI papers**
- **30+ proprietary tools**
- **Board of Directors, ACM SIG Bio**
- 10+ government projects

- **50+ SCI papers**
- **President of the AI Society, KIISE (2017-2019)**
- Professor, Dept. of Computer Science and Engineering, SNU
- Dean, School of Informatics and Computing, Indiana University

- **15 SCI papers (2021.07~)**
- **20+ proprietary tools**
- 4 pharma collaborations
- 5 government projects

03 Partnering & Collaboration

AIGENDRUG
artificial intelligence for drug discovery

서비스 개발 및 검증을 위한 *"협력 네트워크 구축"*

<연구개발> 정부 R&D 사업

농촌진흥청 Rural Development Administration
NRF 한국연구재단
KPBMA 한국제약바이오협회

* 국가연구개발과제 2건 수행 중
* 용역과제 1건

<사업협력> CRO 기업

Biotoxtech
QuBEST BIO

* 큐베스트바이오 업무협약(MOU)

<서비스개발> 대학 연구소

- 서울대 생명공학공동연구원/컴퓨터연구소
- 부산대 AI대학원 인공지능 융합연구센터

* 산학연구계약 5건
* 업무협약(MOU) 2건

<주요고객> 국내 제약사

팜젠사이언스
GC녹십자
TXINNO BIOSCIENCE

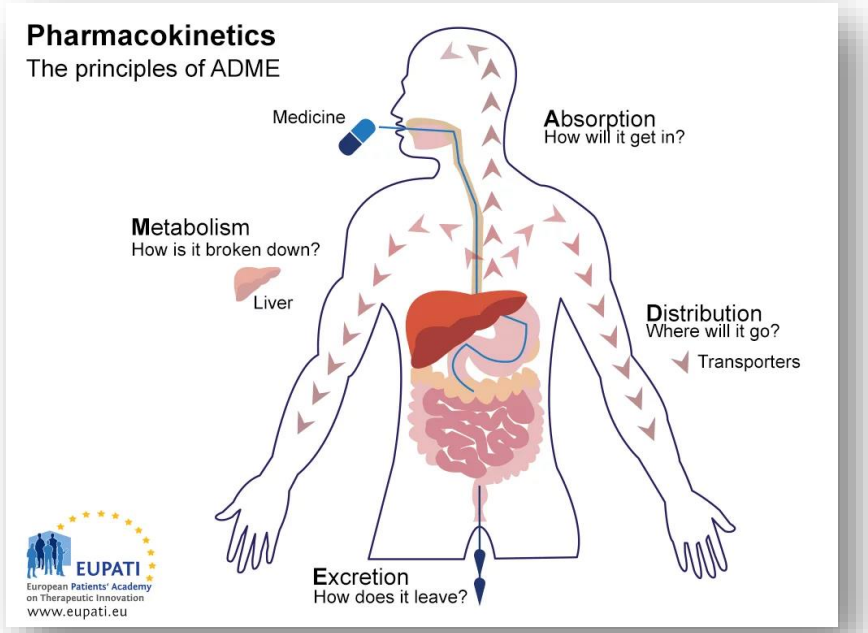
* 공동연구 서비스 계약 3건

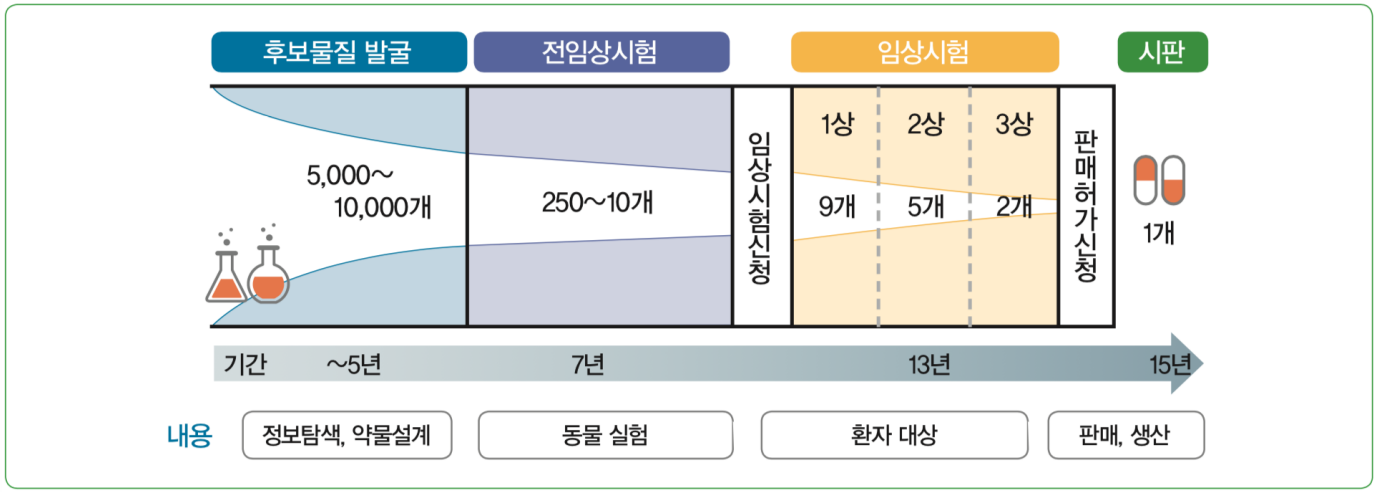
04 프로젝트 배경

AIGENDRUG
artificial intelligence for drug discovery

- 자연계의 화합물(Compound) 중 약물 (Drug)으로 개발되는 비율은 극소수
  - 약효의 존재여부
  - 흡수(Absorption), 분포(Distribution), 대사(Metabolism), 배설(Excretion), 독성(Toxicity) 의 적합성

- 다수의 화합물이 약효가 뛰어남에도, ADMET의 부적합성으로 인하여 약물로 개발에 실패함





AIGENDRUG
artificial intelligence for drug discovery

- **개발 내용**

  본 과제에서는 화합물의 ADMET 정보가 담겨있는 데이터베이스를 기반으로, 화합물 기반 인공지능 기술을 활용하여 다양한 화합물의 성질을 예측하고 약물 적합도 (drug-likeness)를 평가하는 알고리즘 개발을 목적으로 함

  1. 화합물에 적용가능한 인공지능 기법의 이해
  2. 화합물 및 약물 적합도(drug-likeness) 관련 데이터의 이해
  3. 화합물 구조를 기반으로 약물 적합도를 예측하는 알고리즘의 개발

Chemical tasks in drug discovery. The data imported from [12]. (Binary: Binary classification, Reg: Regression)

Task	Dataset	Size	ML Type	Reference
Absorption	Caco-2 (Cell Effective Permeability)	910	Reg	[17]
	HIA (Human Intestinal Absorption)	578	Binary	[18]
	Pgp (P-glycoprotein) inhibition	1,218	Binary	[19]
	Bioavailability	640	Binary	[20]
	Lipophilicity	4,200	Reg	[11]
	Solubility	9,982	Reg	[21]
	Hydration Free Energy	642	Reg	[11,22]
	Subtotal	16,558		
Distribution	BBBP (Blood–Brain Barrier Permeability)	1,975	Binary	[11,23]
	PPBR (Plasma Protein Binding Rate)	1,797	Reg	[24]
	VDss (Volume of Distribution at steady state)	1,130	Reg	[25]
	Subtotal	4,678		
Metabolism	CYP P450 - 2C19 Inhibition)	12,665	Binary	[26]
	CYP P450 - (2D6 Inhibition)	13,130	Binary	[26]
	CYP P450 - (3A4 Inhibition)	12,328	Binary	[26]
	CYP P450 - (1A2 Inhibition)	12,579	Binary	[26]
	CYP P450 - (2C9 Inhibition)	12,092	Binary	[26]
	CYP2C9 Substrate	666	Binary	[27,28]
	CYP2D6 Substrate	664	Binary	[27,28]
	CYP3A4 Substrate	667	Binary	[27,28]
	Subtotal	16,877		
Excretion	Half Life	667	Reg	[29]
	Clearance (microsome)	1,102	Reg	[24,30]
	Clearance (hepatocyte)	1,020	Reg	[24,30]
	Subtotal	1,592		
Toxicity	LD50	7,385	Reg	[31]
	hERG blockers	648	Binary	[32]
	hERG Central	306,893	Binary/Reg	[33]
	Ames Mutagenicity	7,255	Binary	[34]
	DILI (Drug-Induced Liver Injury)	475	Binary	[35]
	Skin reaction	404	Binary	[36]
	Carcinogens	278	Binary	[28,37]
	Tox21	7,831	Binary	[38]
	ToxCast	8,576	Binary	[39]
	ClinTox	1,484	Binary	[40]
	Subtotal	327,133		
	Total	349,036		

Lim, Sangsoo, et al. "On modeling and utilizing chemical compound information with deep learning technologies: A task-oriented approach." *Computational and Structural Biotechnology Journal* (2022).

AIGENDRUG

artificial intelligence for drug discovery

서울시 관악구 관악로1, 220동 630-2호
Tel. 010-2516-9716 | Fax 0504-073-2308