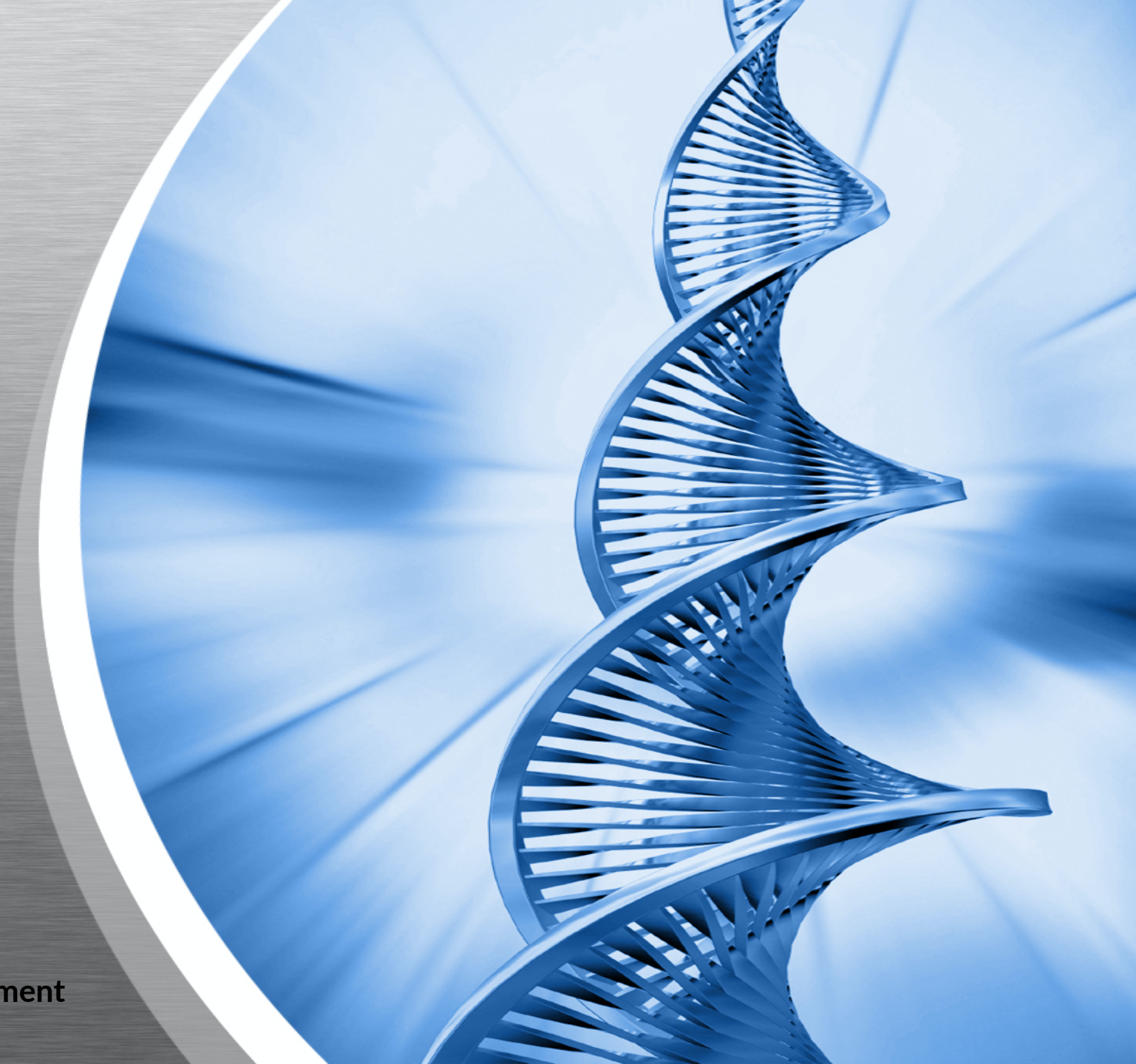


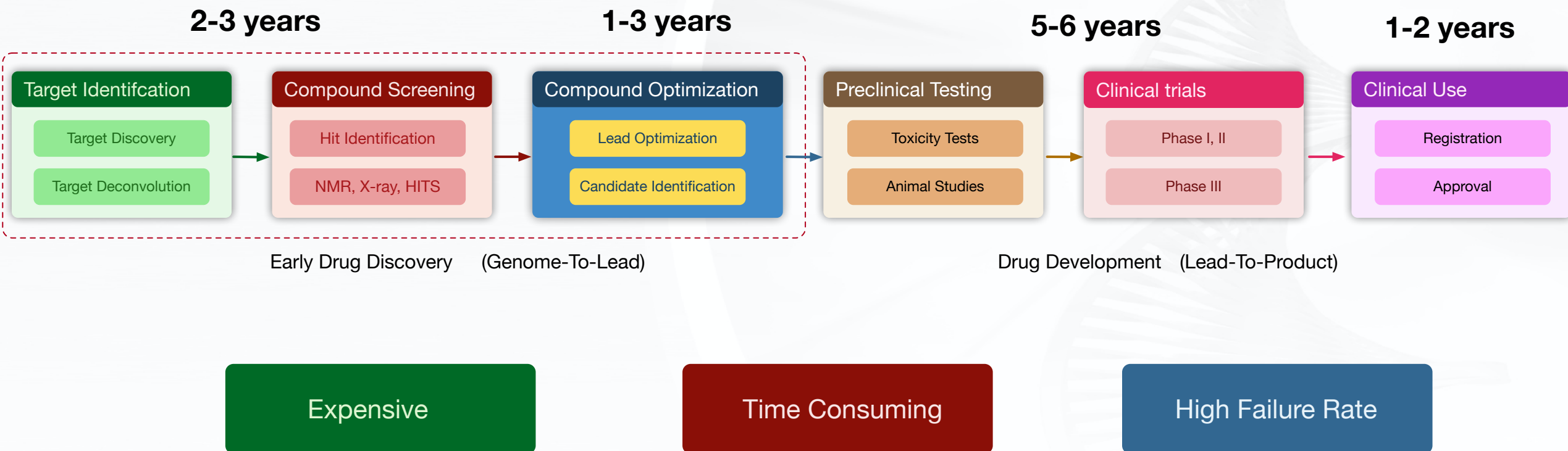
# ORIENTATION

Korea AI Center for Drug Discovery and Development



# Drug Discovery

- Developing and discovering a new drug is a very costly and time consuming process, which can take ~12 years with a cost of 2.8\$ billion dollar



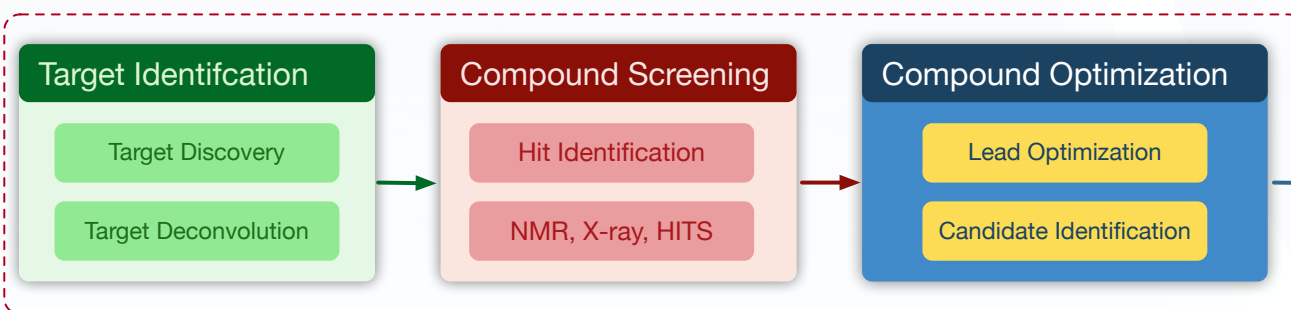
# AI Driven Drug Discovery



SPOTLIGHT · 30 MAY 2018

## How artificial intelligence is changing drug discovery

Machine learning and other technologies are expected to make the hunt for new pharmaceuticals **quicker**, **cheaper** and more **effective**

**0.5 – 1 year**

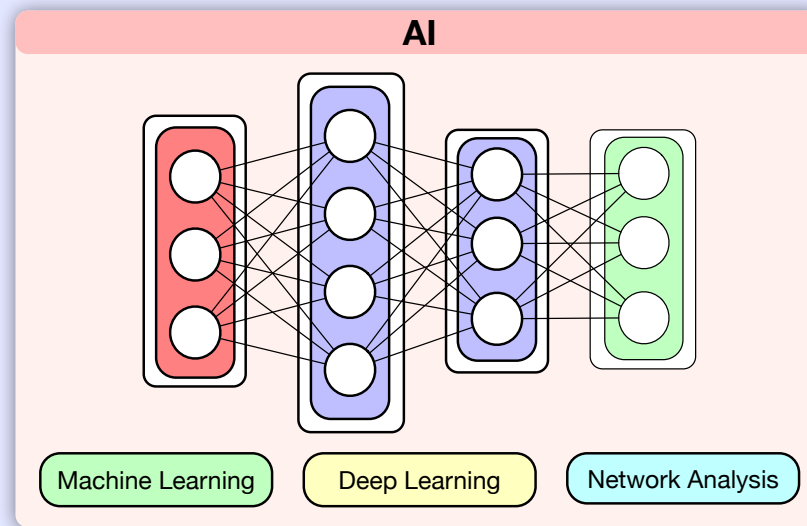
Early Drug Discovery (Genome-To-Lead)

**3 years**

Drug Development (Lead-To-Product)

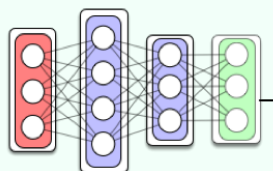
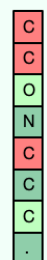
**1-2 years**

# AI DRIVEN DRUG DISCOVERY



## Molecular Property Prediction

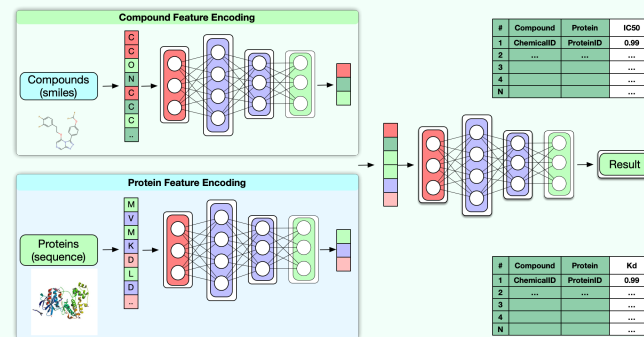
Representation



ESOL  
QSAR  
+  
Toxicity

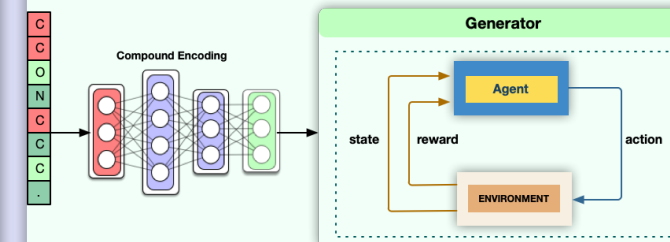
일반교육 Day 2

## Drug Target Interaction



일반교육 Day 3

## De Novo Drug Design



일반교육 Day 3, 전문교육



# Agenda

시간	제목	내용
09:00~09:40	Introduction	Introduction, QSAR Modeling
10:00~10:40	EDA with Jupyter	Rdkit, ChEMBL DB
11:00~11:40	AI basic	실습에 필요한 이론, 알고리즘
12:00~13:00	점심시간	
13:00~13:40	QSAR Modeling (Deepchem)	Solubility Modeling(DeepChem)
14:00~14:40	QSAR Modeling (Prediction Modeling using Pytorch)	Solubility Modeling: Prediction(DNN)
15:00~15:40		GPU usage & Hyperparameter turning
16:00~16:40		Solubility Modeling: Prediction(CNN, Mol2Vec)
17:00~17:40	QSAR Modeling (Classification Modeling using Pytorch)	Penetration Modeling: Binary Classification