ORIENTATION

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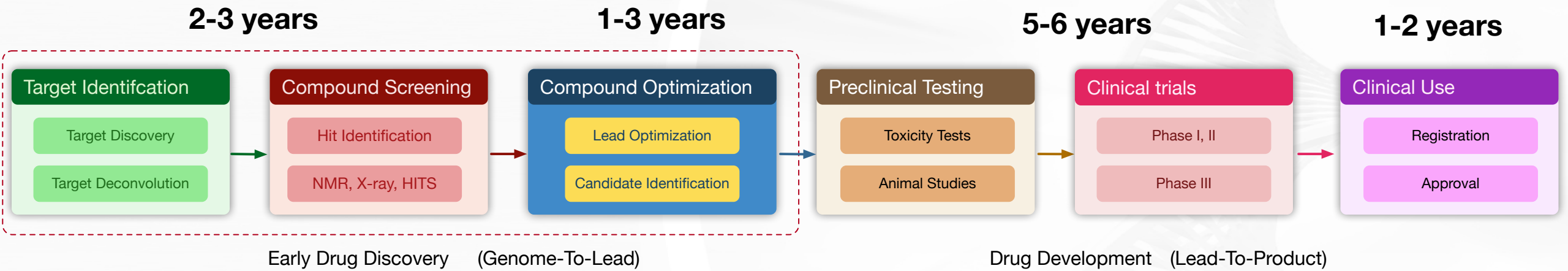
Drug Discovery

- 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



Expensive

Time Consuming

High Failure Rate

AI Driven Drug Discovery

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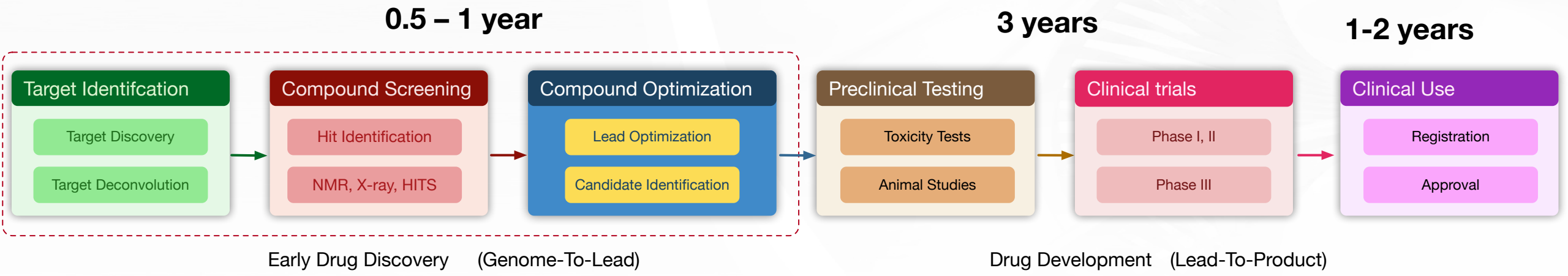
SPOTLIGHT · 30 MAY 2018

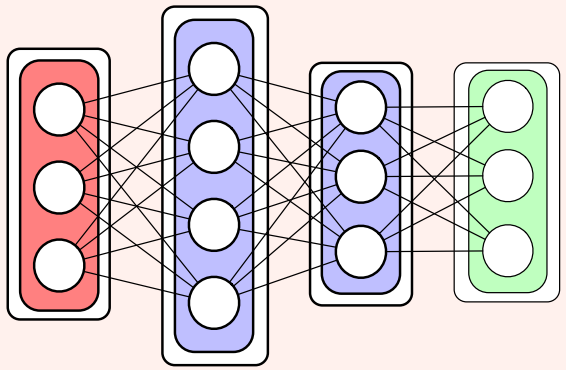
How artificial intelligence is changing drug discovery

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



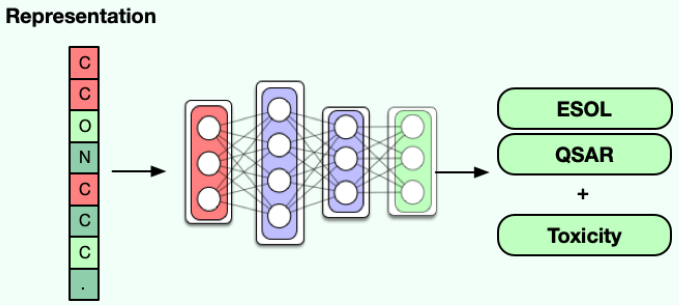
AI DRIVEN DRUG DISCOVERY

AI



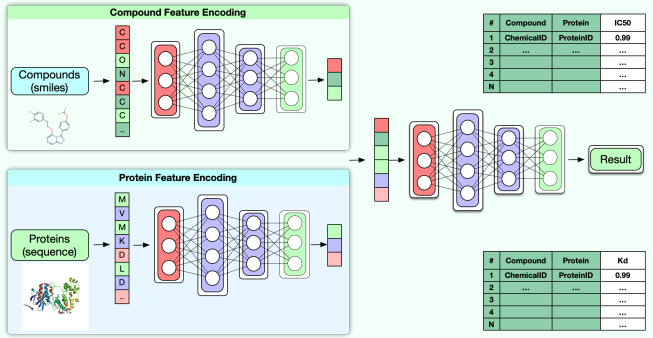
Machine Learning | Deep Learning | Network Analysis

Molecular Property Prediction



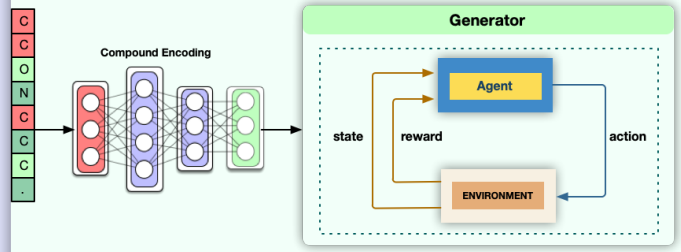
일반교육 Day 2

Drug Target Interaction



일반교육 Day 3

De Novo Drug Design



일반교육 Day 3, 전문교육

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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 15:00~15:40	QSAR Modeling (Prediction Modeling using Pytorch)	Solubility Modeling: Prediction(DNN) 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