KNOWLEDGE-AUGMENTED GRAPH MACHINE LEARNING FOR DRUG DISCOVERY: FROM PRECISION TO INTERPRETABILITY

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OUTLINE

I. Introduction and Motivation
II. Background of Drug Discovery
III. Graph Machine Learning (GML) and Knowledge Graph (KG) in Drug Discovery
IV. Knowledge-augmented Graph Machine Learning (KaGML) for Drug Discovery
V. Practical Resources
VI. Open Challenges and Future Directions

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SIGNIFICANCE AND CHALLENGES OF DRUG DISCOVERY

DRUG DISCOVERY IS LONG AND EXPENSIVE

- It usually takes 10-15 years and costs around 2 billion US dollars

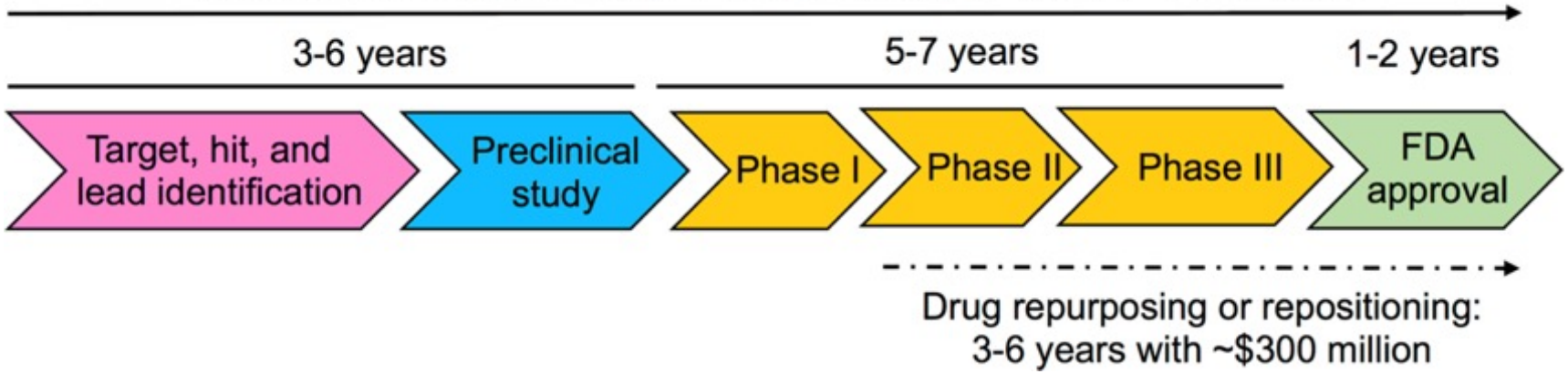
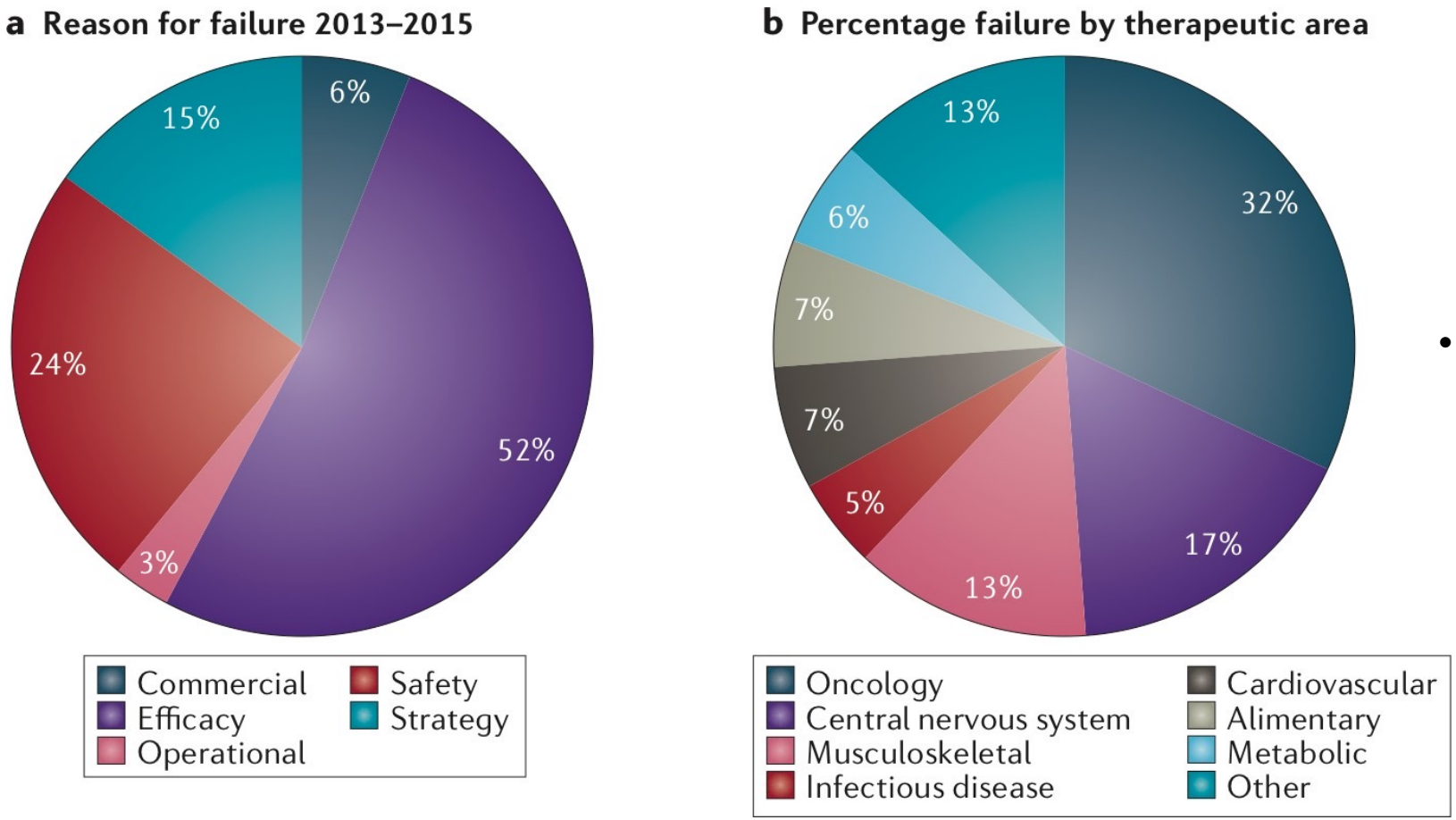


Figure Source: *Cheng F.*, Methods Mol. Biol., 2019

REASONS FOR DRUG DISCOVERY FAILURES

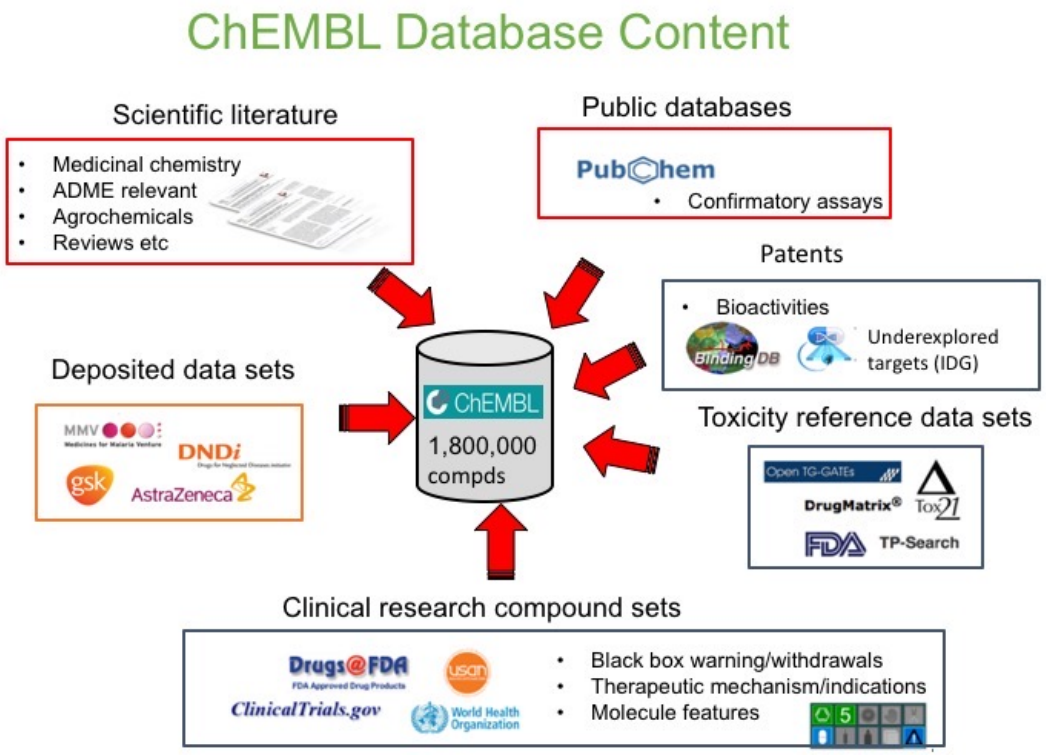


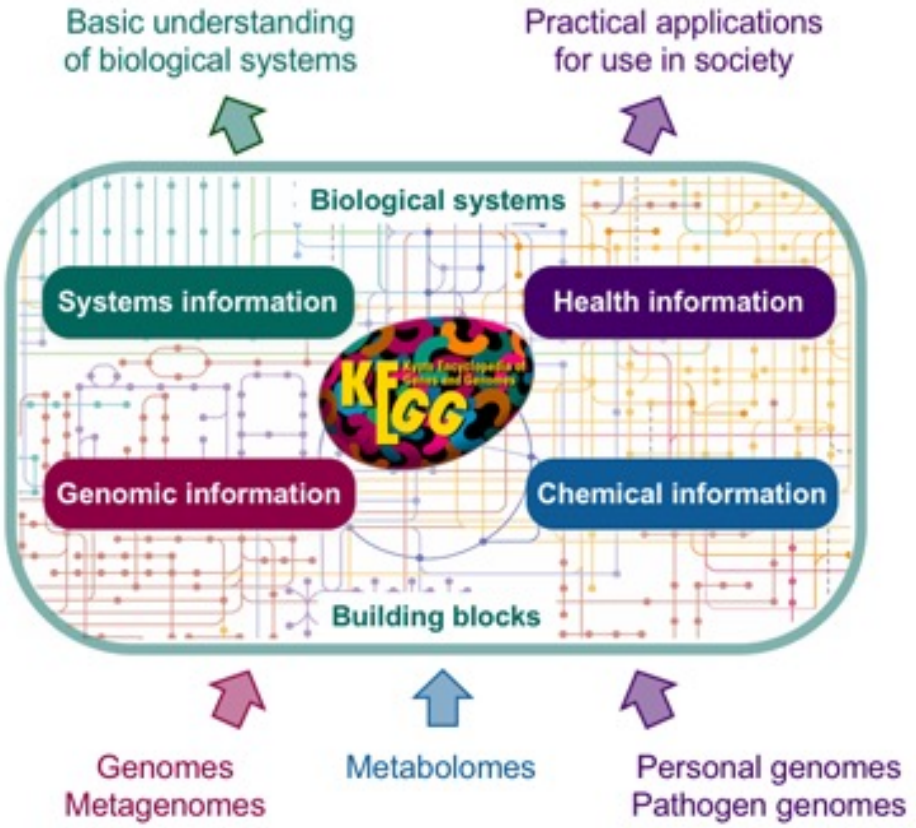
- AI techniques can potentially address major failures.

Figure Source: *Harrison RK.*, Nat Rev Drug Discovery 2020

BIG OPPORTUNITY FOR AI

- A huge amount of data is generated in the biomedical domain





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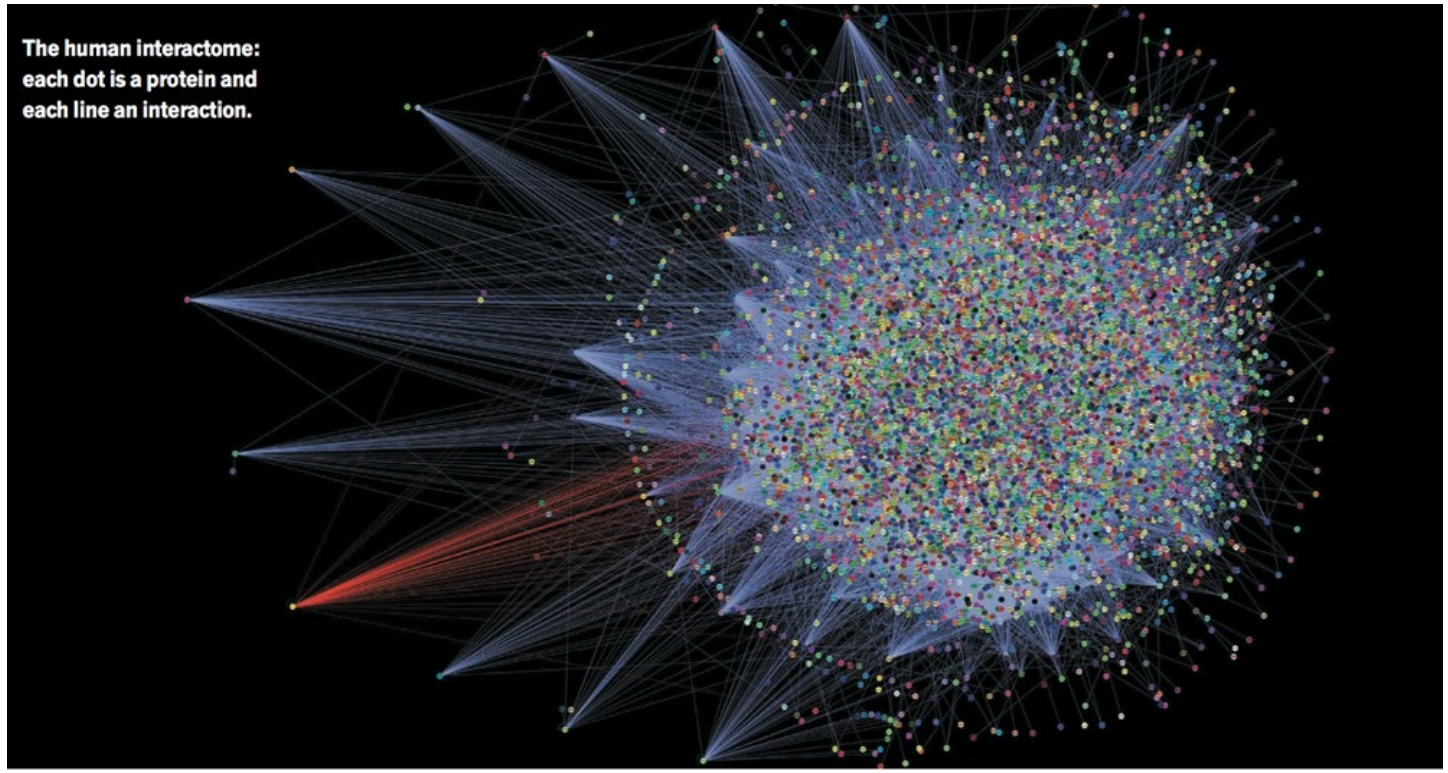


Fessenden et al., Nature 2017

Luck et al., Nature 2020

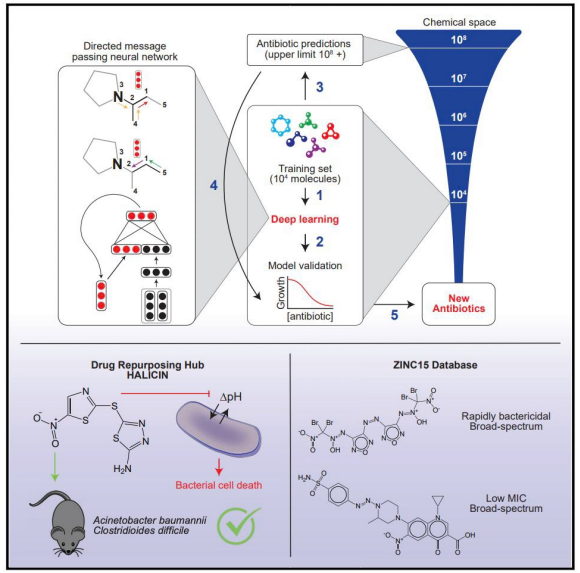
- ~13 major organ systems
- ~200-300 cell types
- ~10-50 trillion total human cells
- ~20,000 protein-coding genes
- ~3,000 metabolites
- ~300 different post-translational modifications
- ~600K binary interactions of proteins
- Over 2M nodes among # DNA, RNA, protein and variants

PROMISING AI IN DRUG DISCOVERY

Cell

A Deep Learning Approach to Antibiotic Discovery

Graphical Abstract



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Highly accurate protein structure prediction with AlphaFold

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Thank you!

Questions?

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