Machine Learning for Drug Development

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HARVARD MEDICAL SCHOOL

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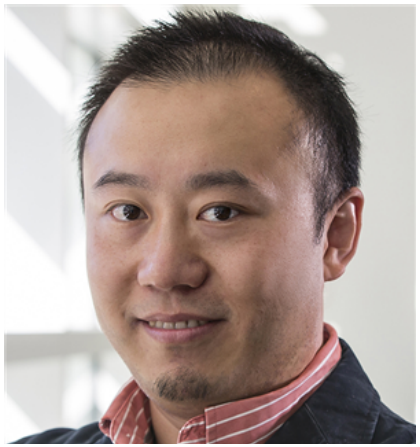
Welcome to our Tutorial!

Marinka Zitnik
Harvard University

Cao (Danica) Xiao
IQVIA



Jimeng Sun
UIUC

Logistics

- IJCAI (https://ijcai20.org):
  - Jan 6, 7-10:15pm Eastern Standard Time
  - Jan 7, 12-3:15pm UTC
  - Jan 7, 9am-12pm Japanese Standard Time
- Location: Red wing, North 3
- Q&A: Use Zoom features

Tutorial website with materials, demos and pointers to code and data resources:

https://zitniklab.hms.harvard.edu/drugml

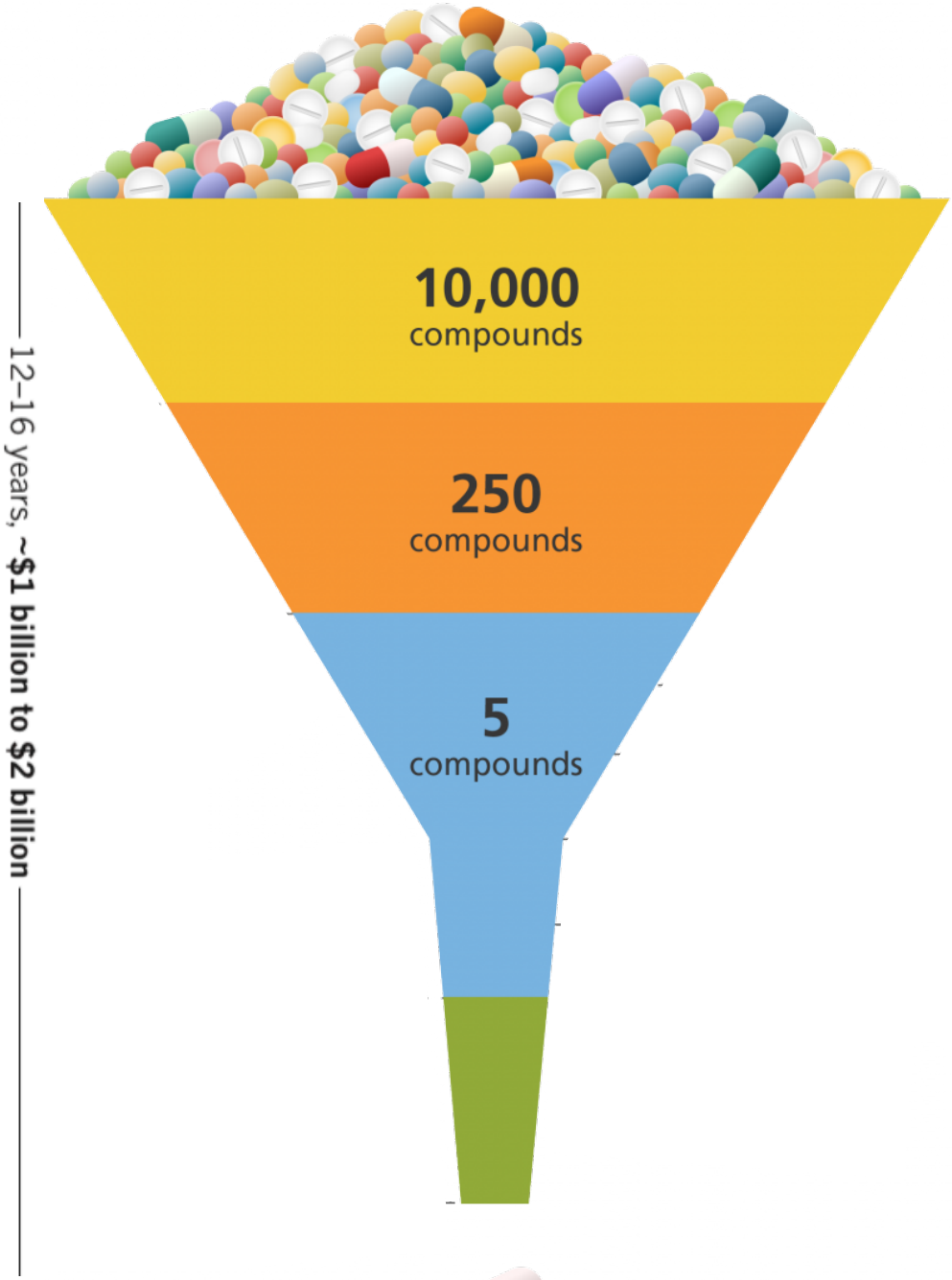
Step 1: Design and Discovery

Step 2: Preclinical Research

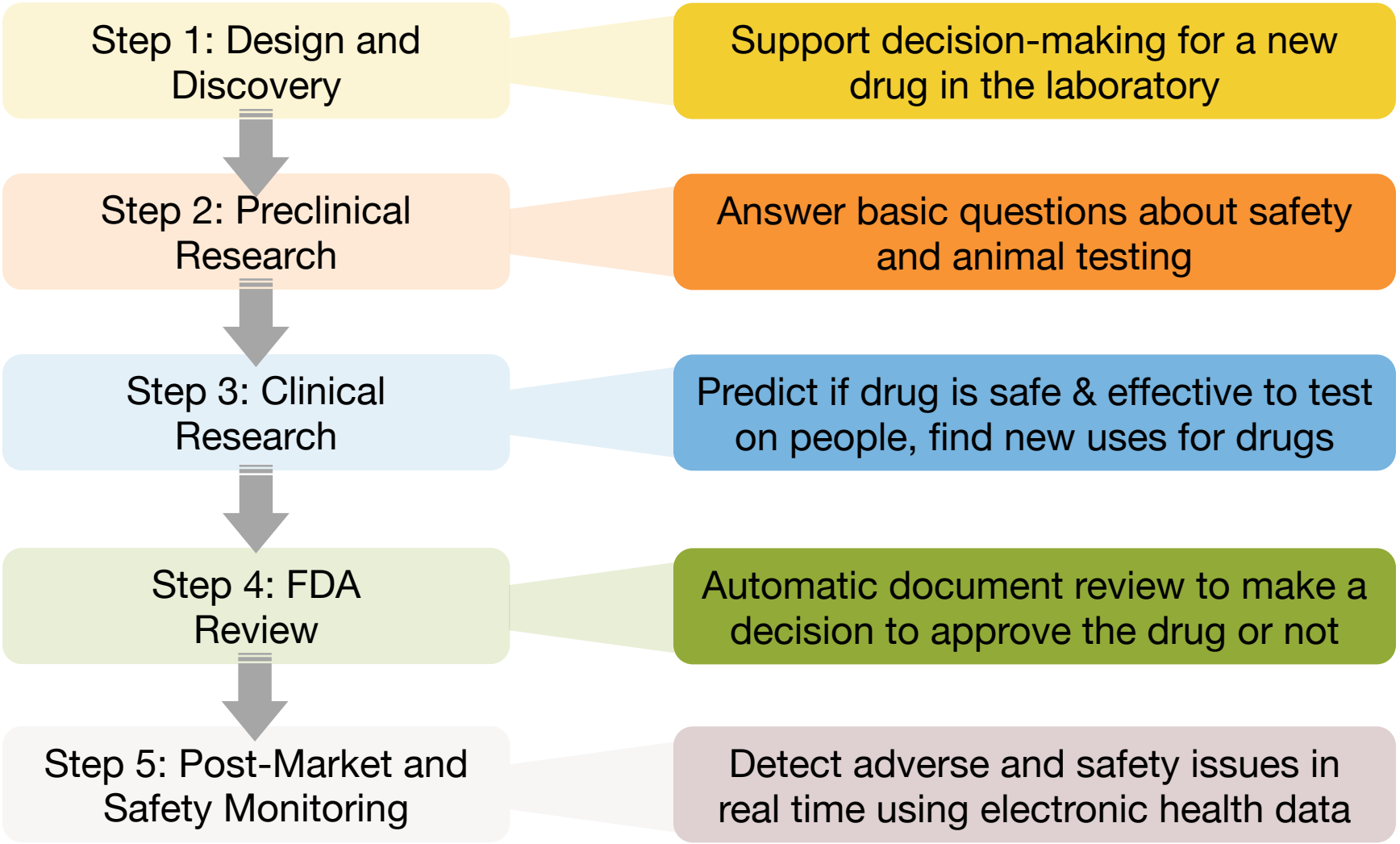
Step 3: Clinical Research

Step 4: FDA Review

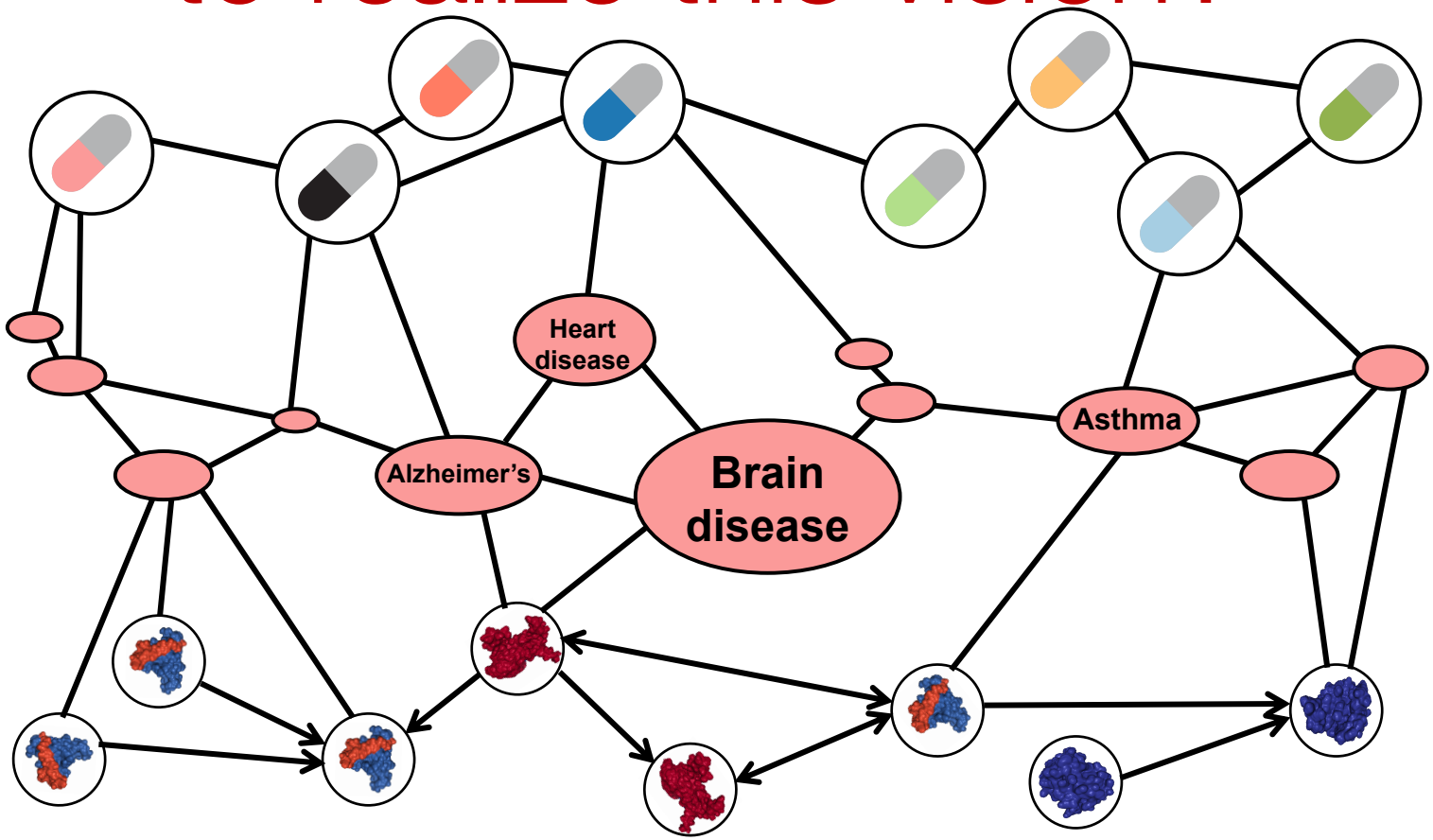
Step 5: Post-Market and Safety Monitoring



Opportunities for AI in Drug Development



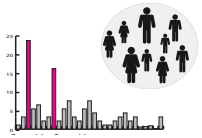
Why is it so challenging to realize this vision?



Finding promising therapeutic interventions for diseases depends on complex interactions, *e.g.,* drug-target, protein-protein, drug-drug, drug-disease, disease-protein dependencies

Why is it so challenging to realize this vision?

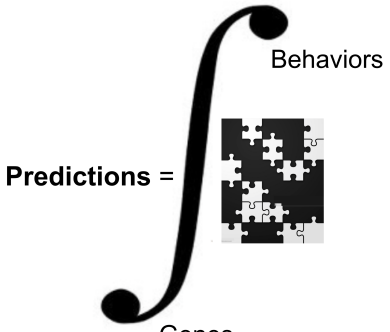
Need to integrate heterogeneous, confounded data that **span from molecules to society**



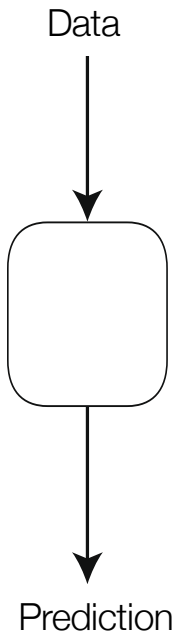
Genome

Health records

Behaviors, lifestyle, vital signs



Need to translate predictions into **actionable** hypotheses



Multi-scale: molecules, individuals, populations

Heterogeneous: experimental readouts, curated, self-reported

Confounded: data from different technologies, and measurement platforms

Outline

Overview and introduction

Part 1: Virtual drug screening and drug repurposing

Part 2: Adverse drug effects, drug-drug interactions

Part 3: Clinical trial site identification, patient recruitment

Part 4: Molecule optimization, molecular graph generation, multimodal graph-to-graph translation

Part 5: Molecular property prediction and transformers

Demos, resources, wrap-up & future directions

Let’s begin!