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# Dr. Data: An Integrated Drug Repurposing Database for Identifying New Indications of FDA Approved Drugs

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## ❖ Priority Areas

### Section 5. Harness Diverse Data through Information Sciences to Improve Health Outcomes: Strategic Plan for Regulatory Science

1. Enhance information technology infrastructure development and data mining:
  - a) **Improve access to large, complex data sets** to solve problems faster or to allow solutions of otherwise intractable problems (e.g., multi-dimensional map of Salmonella);
2. Develop and apply simulation models for product life cycles, risk assessment, and other regulatory science uses:
  - b) **Promote novel clinical trial design** using simulation, new statistical models, and novel animal models/animal model alternatives.

### Section 2. Stimulate Innovation in Clinical Evaluations and Personalized Medicine to Improve Product Development and Patient Outcomes: Strategic Plan for Regulatory Science

3. Identify and qualify biomarkers and study endpoints:
  - b) Develop and evaluate novel approaches for **biomarker identification**, including 'omics, systems biology, and high throughput methods;

## ❖ Drug Repurposing

- The process of identifying new indications for previously approved drugs
- Reduced cost and the potential for rapid clinical transition (versus \$2.5B and >14 years to develop a new drug)
- Low and high throughput screening of FDA approved compound library against disease specific assays

## ❖ Current Drug Repurposing Effort: New Therapeutic Uses Projects

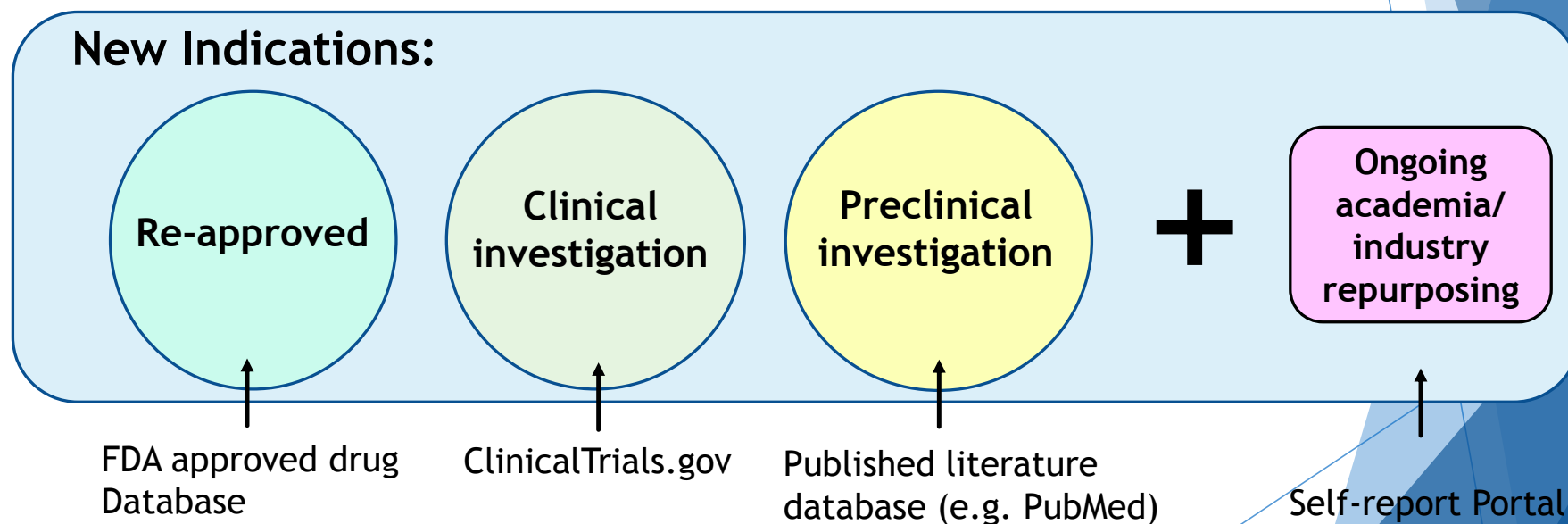
National Center for Advancing Translational Sciences (NCATS):

- NIH-Industry Partnerships Initiative (AstraZeneca, Janssen, Pfizer, AbbVie, etc.)
  - Launched in May 2012
  - Foster collaboration between pharmaceutical companies and the biomedical research community
- Bench-to-Clinic Repurposing Initiative
  - Funding opportunities to support pre-clinical and clinical studies

**The access to large, complex drug repurposing data sets has not been readily available**

## ❖ Solution: Dr. Data: Collaborative Information Database on Drug Repurposing

Molecular, literature-derived and clinical data: structures and drug targets

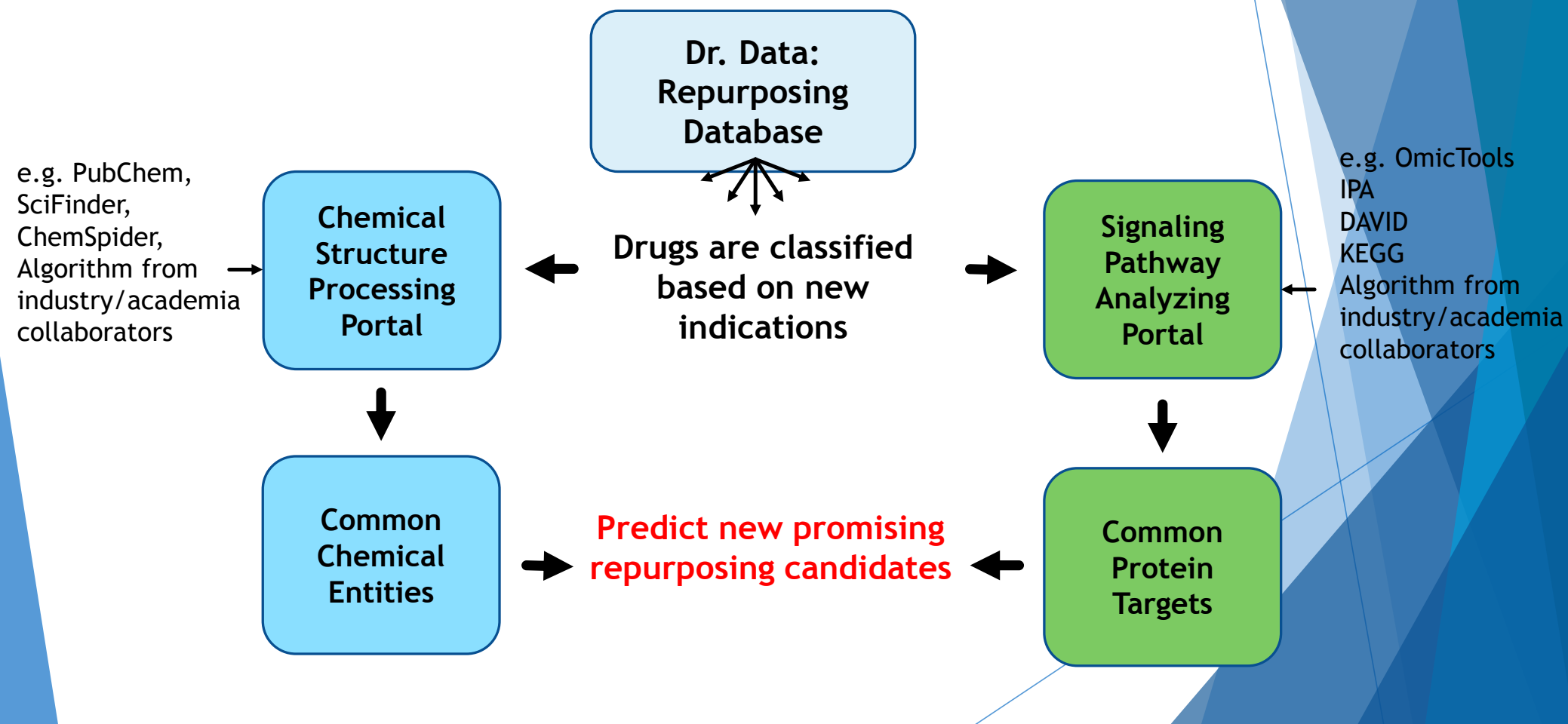


\*\*Exclude drugs under active recalls

## ❖ **Solution: Dr. Data: Collaborative Information Database on Drug Repurposing**

- **Data will be annotated using meta-analysis to allow easy access to references**
- **Data harmonization and transparency: OpenFDA portal offers standard data format for quick and easy application**
- **Dr. Data will be implemented with appropriate cybersecurity controls**

## ❖ Solution: Analytical Tools Embedding



## ❖ Example: Common Structural Processing and Prediction

Repurposing  
Database



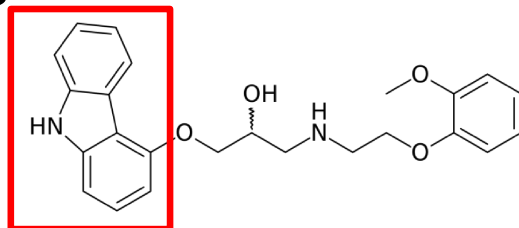
Chosen new indication: Anticancer

### Carvedilol

Brand name: Coreg

Beta blocker used  
to treat **congestive  
heart failure**

New indication: under  
preclinical investigation

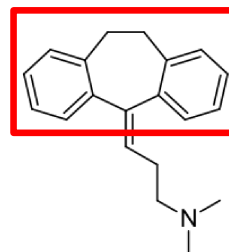


### Amitriptyline

Brand name: Elavil

Antidepressant used to  
treat **major depression  
disorder**

New indication: under clinical  
investigation





# ❖ Example: Common Structural Processing and Prediction

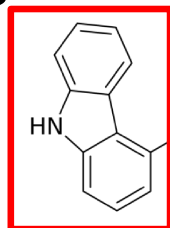
Repurposing Database

## Carvedilol

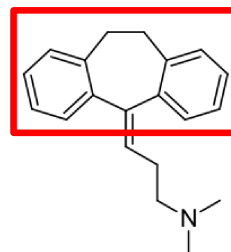
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Chosen new indication: Anticancer



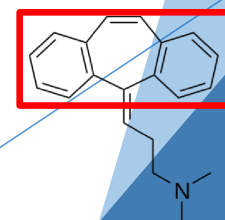
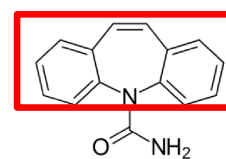
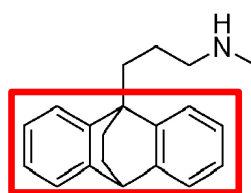
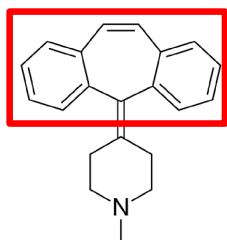
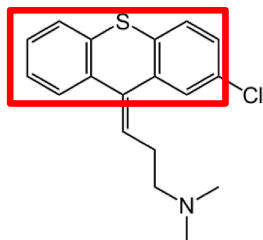
## Amitriptyline

Brand name: Elavil

Antidepressant used to treat **major depression disorder**

New indication: under clinical investigation

Prediction: drugs with a common tricyclic structure (similarity threshold: >90%)



## ❖ Why Do we Care?

- Exciting preclinical research directions, new biomarkers and novel clinical trials
- Identify potential treatment for rare diseases
- Collaboration between industry, government agencies and academia
- Insights on trends in the drug discovery field
- \$\$\$

**Questions?**

