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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

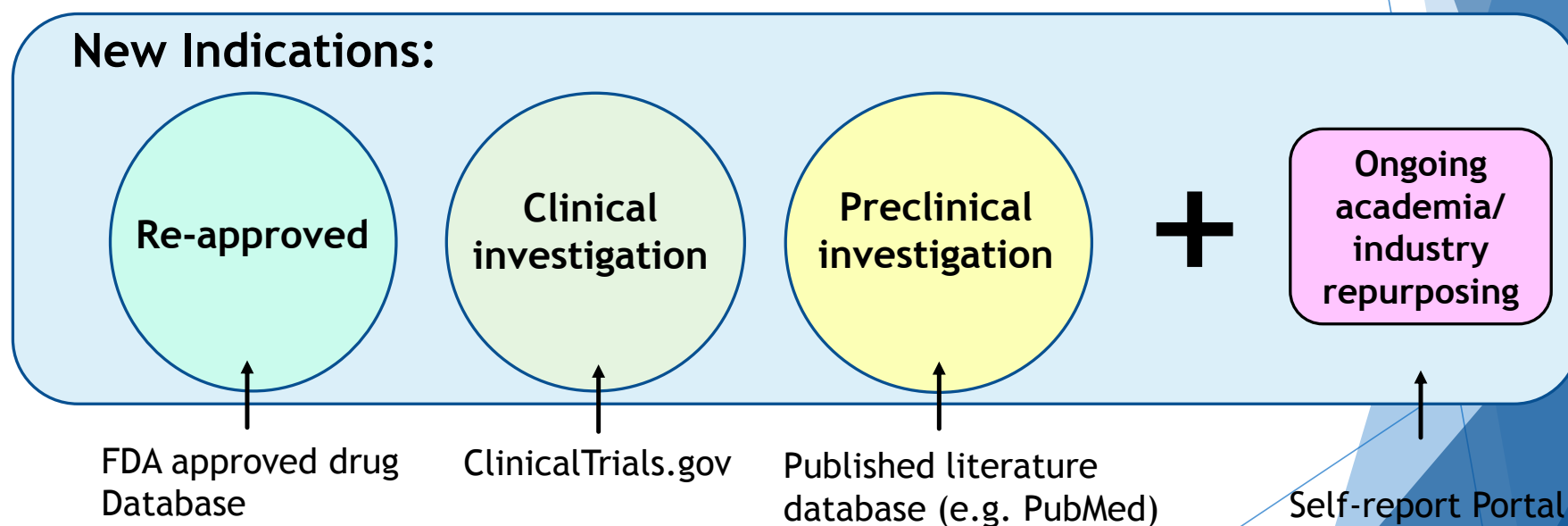
National Center for Advancing Translational Sciences NCATS :

- 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

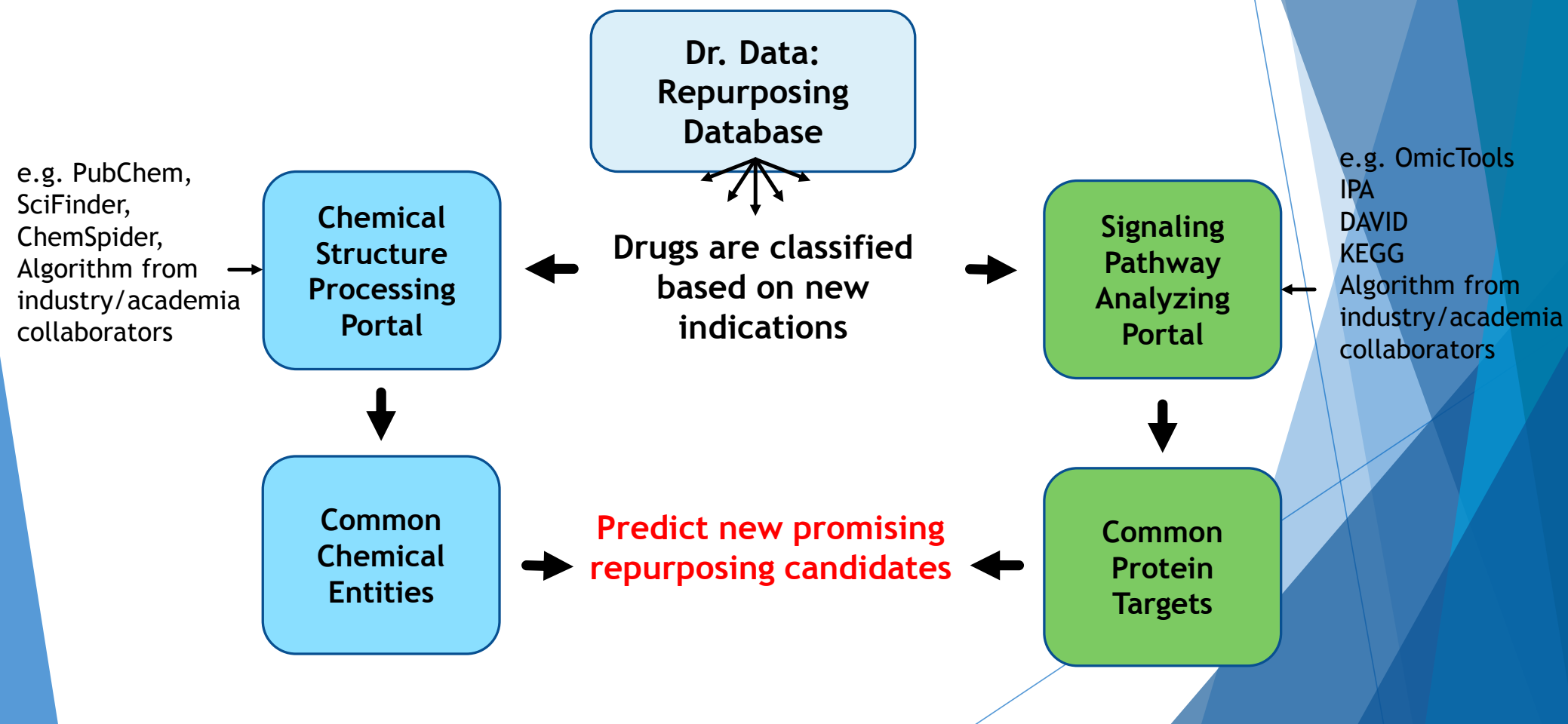


**Exclude drugs under active recalls

❖ **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



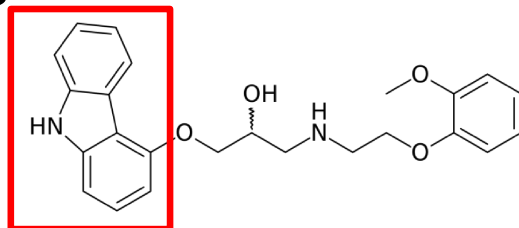
Chosen new indication: Anticancer

Carvedilol

Brand name: Coreg

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

New indication: under
preclinical investigation

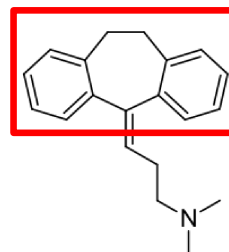


Amitriptyline

Brand name: Elavil

Antidepressant used to
treat **major depression
disorder**

New indication: under clinical
investigation



❖ Example: Common Structural Processing and Prediction

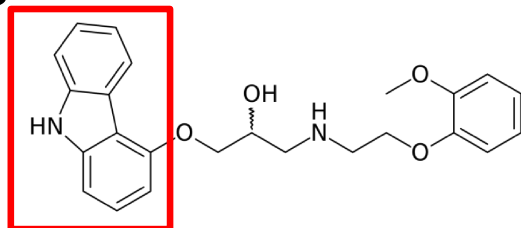
Repurposing Database

Carvedilol

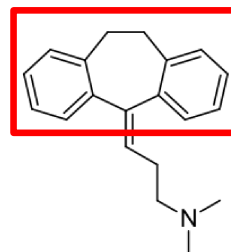
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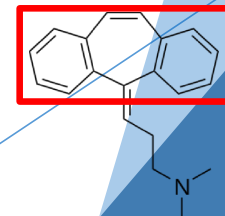
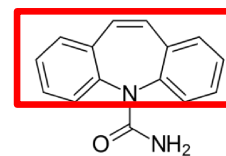
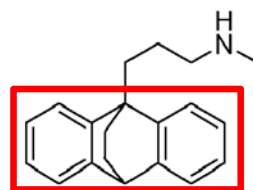
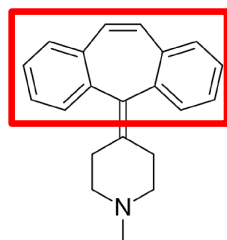
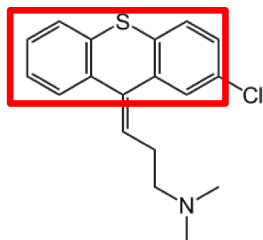
Amitriptyline

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?

