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

**New Indications:**
- Re-approved
  - FDA approved drug Database
- Clinical investigation
  - ClinicalTrials.gov
- Preclinical investigation
  - Published literature database (e.g. PubMed)

**Ongoing academia/industry repurposing**
- Self-report Portal

**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

Dr. Data: Repurposing Database

Drugs are classified based on new indications

Chemical Structure Processing Portal

Common Chemical Entities

Predict new promising repurposing candidates

Signaling Pathway Analyzing Portal

Common Protein Targets

e.g. PubChem, SciFinder, ChemSpider, Algorithm from industry/academia collaborators

e.g. OmicTools IPA DAVID KEGG Algorithm from industry/academia collaborators
Example: Common Structural Processing and Prediction

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
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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?