where are there databases of drug repurposing

The exploration and utilization of databases for drug repurposing are critical in identifying new uses for existing drugs, which can potentially reduce costs and accelerate drug development. Here's a summary of the evidence from the provided articles regarding the databases that support drug repurposing:

* The article by Tanoli et al. [3] provides a comprehensive survey of 102 databases that are instrumental in drug repurposing efforts. These databases are categorized into four main types based on the data they offer, which include chemical, biomolecular, drug-target interaction, and disease databases. This categorization helps in designing computational pipelines for drug repurposing and facilitates the creation of novel drug repurposing pipelines through machine learning methods.

* CADDIE, as described by Hartung et al. [2], is another significant resource. It integrates six human gene-gene and four drug-gene interaction databases, along with information on cancer driver genes, mutation frequencies, gene expression data, and anticancer drugs. This tool aids in the identification of drug targets and repurposing candidates in oncology through a user-friendly web interface and various network algorithms.

These databases and tools are essential for harnessing the vast amount of drug-related data available, helping researchers and clinicians to efficiently identify potential new therapies for various diseases, especially in cases where traditional drug development may be limited or slow.

References:
[2] Hartung M, Anastasi E, Mamdouh ZM, et al. Cancer driver drug interaction explorer. Nucleic Acids Res. 2022;50(W1):W138-W144.
[3] Tanoli Z, Seemab U, Scherer A, et al. Exploration of databases and methods supporting drug repurposing: a comprehensive survey. Briefings in Bioinformatics. 2021;22(2):1656-1678.

Citation Summaries

Citation: [2] Hartung M, Anastasi E, Mamdouh ZM, et al. Cancer driver drug interaction explorer. Nucleic Acids Res. 2022;50(W1):W138-W144.

Summary:

1. **Purpose**

- **Objective** : To address challenges in targeted cancer therapy by developing CADDIE, a tool that aids in drug repurposing and identification of drug targets using network medicine algorithms.
- **Methods** : Integration of six human gene-gene and four drug-gene interaction databases, and various other resources like cancer driver genes data, mutation frequencies, and gene expression data. CADDIE utilizes seven different network algorithms to analyze this integrated data for identifying drug targets and repurposing candidates.

2. **Main Conclusions**

- CADDIE enables the identification and prioritization of drug targets and repurposing candidates in oncology through a user-friendly web interface that integrates extensive genomic and drug data. It simplifies the complex data and network analysis processes, making these accessible to a broader range of researchers, including those without advanced computational skills.

3. **Risks**

- No specific risks like addiction or death were mentioned in relation to the use of CADDIE. However, the general risks associated with cancer drug therapy such as side effects and drug resistance were noted.

4. **Benefits**

- Facilitates the rapid and cost-effective identification of new uses for existing drugs.
- Provides a comprehensive visualization and interactive analysis of gene and protein interactions, aiding in the understanding and exploration of complex cancer-related data.
- Enhances the reproducibility and transparency of research through detailed documentation of analysis parameters and results.

5. **Search Methodology and Scope**

- The tool integrates multiple databases and sources, covering a broad spectrum of gene-gene and drug-gene interactions, mutation frequencies, and gene expression data specific to various cancer types. This comprehensive integration ensures that the scope of the literature and data included is extensive and relevant to the field of oncology.

6. **Selection Criteria**

- Studies and datasets included are those related to gene-gene interactions, drug-gene interactions, cancer driver genes, and mutation frequencies among others. The selection seems to focus on high-quality, peer-reviewed sources, ensuring reliability but it is not explicitly mentioned how contradictory findings or alternative theories are addressed.

7. **Quality Assessment of Included Studies**

- Although the specific methods for quality assessment of the included studies are not detailed, the use of reputed databases and peer-reviewed sources suggests a focus on high-quality data.

8. **Synthesis and Analysis**

- Utilizes network-based algorithms to synthesize and analyze the data. The algorithms include propagation methods and aggregation approaches, which help in identifying both direct and indirect drug targets. The synthesis appears structured and methodologically sound, although specific statistical metrics like p-values or effect sizes are not mentioned.

9. **Sources of Funding or Conflict of Interest**

- Funded by the European Union’s Horizon 2020, the German Federal Ministry of Education and Research, and other institutional and personal grants. No conflicts of interest were declared, suggesting an unbiased approach to the research and development of CADDIE.

PMID: 35580047

PMCID: PMC9252786

URL: https://pubmed.ncbi.nlm.nih.gov/35580047/

Citation: [3] Tanoli Z, Seemab U, Scherer A, et al. Exploration of databases and methods supporting drug repurposing: a comprehensive survey. Briefings in Bioinformatics. 2021;22(2):1656-1678.

Summary:

1. **Purpose**

- **Addressing Issue** : The review addresses the challenges in drug repurposing, particularly the issue of selecting appropriate databases from a large number available, which contain relevant drug-related data for hypothesis building.
- **Method Used** : The review provides a survey of 102 databases, categorizing them into four main types based on the data they offer, and discusses how these databases can be used for drug repurposing.

2. **Main Conclusions**

- **Conclusions** : The review concludes that the surveyed databases can significantly aid in designing computational pipelines for drug repurposing by providing necessary data and facilitating the creation of novel drug repurposing pipelines through machine learning methods.
- **Implications** : The ability to effectively use these databases can accelerate the identification of new uses for existing drugs, enhancing the drug development process and potentially reducing costs and time-to-market for repurposed drugs.

3. **Risks**

- **Mentioned Risks** : The main limitations mentioned include data heterogeneity and the overabundance of variables relative to the number of samples, which can affect the accuracy and effectiveness of drug repositioning efforts using machine learning.

4. **Benefits**

- **Purported Benefits** : Benefits include the potential for accelerated drug repurposing, cost reduction in drug development, and the identification of new drug uses, particularly for orphan diseases where traditional drug development is limited.

5. **Search Methodology and Scope**

- **Search Strategy** : The review categorizes and evaluates 102 databases, dividing them into subcategories based on their content and utility in drug repurposing.
- **Scope and Relevance** : The scope is comprehensive, encompassing a wide range of

databases essential for drug repurposing, thus covering a significant portion of available resources.

6. **Selection Criteria**

- **Inclusion/Exclusion** : The review includes databases that are relevant to drug repurposing, categorized into chemical, biomolecular, drug-target interaction, and disease databases.
- **Diversity and Contradictory Findings** : The review appears to include a diverse range of databases but does not explicitly mention how contradictory findings are addressed.

7. **Quality Assessment of Included Studies**

- **Quality Assessment Methods** : The review assesses the databases based on parameters like the number of chemicals, genes, diseases, etc., but specific quality assessment methods for the included studies are not detailed.

8. **Synthesis and Analysis**

- **Synthesis Methodology** : It categorizes the databases into main and subcategories and evaluates them based on their strengths and comprehensiveness.
- **Statistical Tests and Metrics**: The review does not explicitly mention the use of statistical tests or metrics in the analysis of database information.

9. **Sources of Funding or Conflict of Interest**

- **Funding** : Supported by the European Research Council (ERC), Academy of Finland, European Commission H2020 EOSC-life, and Medicinska Understödsföreningen Liv och Hälsa.
- **Conflict of Interest** : No conflicts of interest are mentioned explicitly, although the affiliations of the authors are disclosed.

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PMCID: PMC7986597

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