SECTION 6. PHARMACY

DOI: 10.46299/ISG.2023.MONO.MED.4.6.1

6.1 Beyond traditional applications: repositioning medicines for enhanced health care

In the ever-evolving landscape of healthcare, the concept of drug repositioning has emerged as a powerful strategy to revolutionize the field of medicine [228, 229]. Repositioning, also known as drug repurposing or therapeutic switching, involves identifying new applications for existing medications beyond their original intended use. This approach presents a myriad of opportunities to address unmet medical needs, accelerate the drug development process, and potentially reduce costs associated with bringing new treatments to market [230].

Traditionally, the development of new drugs has been a complex and time-consuming process, often taking many years and substantial financial investment. However, drug repositioning offers a compelling alternative by leveraging the vast library of already approved drugs or compounds with known safety profiles. By exploring alternative therapeutic indications, researchers can unlock hidden potentials and create new treatment options for a range of diseases and conditions.

In the dynamic realm of pharmaceutical research and development, drug repositioning has emerged as a captivating avenue with profound implications for modern medicine. This analysis aims to explore the relevance and significance of drug repositioning, examining its current state and the factors driving its widespread adoption [228]. By understanding the context and motivations behind this innovative approach, we can gain valuable insights into its potential to address pressing medical challenges and reshape the landscape of healthcare.

This approach to drug development has several advantages over traditional methods:

- *addressing unmet medical needs*: one key aspect that underscores the relevance of drug repositioning is its ability to address unmet medical needs [231]. With an ever-increasing demand for effective treatments across a wide range of diseases and conditions, there is a pressing need to discover novel therapeutic options. Repositioning offers a unique opportunity to repurpose existing medications for new indications, potentially bypassing the lengthy and costly process of developing entirely new drugs. By capitalizing on the existing safety data and knowledge about these drugs, researchers can expedite the availability of treatments for patients in dire need.

- *accelerating the drug development process*: the traditional drug development process typically spans several stages, including target identification, preclinical testing, and extensive clinical trials. This process can take up to a decade or more, with high rates of failure and substantial financial investments. In contrast, drug repositioning leverages the vast pool of approved drugs or compounds with established safety profiles, thereby shortening the development timeline. By repurposing drugs, researchers can potentially expedite the translation of discoveries into clinical applications, leading to faster availability of treatments and ultimately benefiting patients worldwide [232].
- *cost-effectiveness and market potential*: the financial aspect of drug development cannot be overlooked when assessing the relevance of drug repositioning. Developing new drugs from scratch requires significant investments, including research and development costs, clinical trial expenses, and regulatory fees. In contrast, repurposing existing drugs offers a potentially more cost-effective alternative. With safety data already established, repurposed drugs can bypass some of the early-stage testing and streamline the regulatory approval process. This not only reduces costs but also enhances the market potential for these medications, making them attractive to pharmaceutical companies and investors.
- *expanding therapeutic possibilities*: Another compelling aspect of drug repositioning is its potential to expand therapeutic possibilities. By exploring alternative indications for existing drugs, researchers can uncover new applications and treatment options. This not only maximizes the value of existing medications but also provides alternative approaches to complex diseases or conditions that may have limited treatment options. Repositioning allows for a broader understanding of a drug's

mechanisms of action, potentially leading to unexpected therapeutic benefits and improved patient outcomes [233].

This review delves into the fascinating world of drug repositioning, exploring the reasons behind its growing popularity, the strategies employed to identify potential repositioning candidates, and the impact it has on healthcare systems. Successful case studies, highlighting the transformative impact of repurposed drugs in various therapeutic areas will present. Furthermore, the challenges and future prospects of drug repositioning, shedding light on the ongoing efforts to harness its full potential will discuss.

In modern medicine, drug repositioning encompasses a variety of strategies and approaches to identify and repurpose existing medications for new therapeutic indications [228, 229, 234-238]. There are some of the main means of drug repositioning:

- *serendipitous discoveries*: Sometimes, drug repositioning occurs by chance when unexpected therapeutic benefits are observed during the clinical use of a drug for a different indication. These serendipitous discoveries may prompt further investigation and eventually lead to the approval of a drug for a new medical condition.
- *data mining and bioinformatics*: Large-scale data mining and analysis of biomedical databases, electronic health records, and genomic data can provide valuable insights into potential associations between drugs and different diseases. Bioinformatics tools and computational models are used to identify patterns, predict drug-disease interactions, and prioritize candidates for further evaluation.
- *target-based approaches*: By understanding the molecular targets and mechanisms of action of existing drugs, researchers can explore their potential relevance to other diseases. This involves investigating the biological pathways and targets involved in both the original indication and the target disease, allowing for the identification of drugs that may have efficacy in the new context.

- *repurposing of failed or discontinued compounds*: Drug candidates that failed in clinical trials or were discontinued by pharmaceutical companies for various reasons can be reevaluated for alternative therapeutic indications. These compounds may have demonstrated safety profiles or known mechanisms of action that make them attractive candidates for repurposing.
- *combination therapies*: Drug repositioning can involve exploring the potential of combining existing medications to create synergistic effects or enhance therapeutic outcomes. By combining drugs with different mechanisms of action, researchers can target multiple disease pathways simultaneously, potentially leading to improved efficacy or reduced side effects.
- *drug repositioning screens*: High-throughput screening methods, such as phenotypic screening or drug repurposing libraries, are used to test existing drugs or compounds against different disease models or cellular assays. These screens aim to identify potential candidates with activity against the target disease, even if they were originally developed for a different purpose.
- *clinical observations and trials*: Observational studies and clinical trials play a crucial role in validating the potential of drug repositioning candidates. These studies involve administering existing drugs to patients with the target disease and evaluating their efficacy, safety, and tolerability. Positive results from well-designed trials can support the repurposing of a drug for a new indication.

Repositional pharmacology plays a pivotal role in the process of drug repositioning, which involves identifying and repurposing existing medications for new therapeutic indications [239, 240]. It focuses on understanding the pharmacological properties of drugs and their mechanisms of action to assess their potential efficacy and safety in alternative disease contexts. Here are some key aspects of repositional pharmacology in drug repositioning:

- *mechanistic understanding*: Repositional pharmacology starts with a deep understanding of the drug's mechanism of action in its original indication. This includes knowledge of its target receptors, enzymes, signaling pathways, and interactions with biological systems. By comprehending the underlying pharmacological mechanisms, researchers can explore whether these mechanisms are relevant and applicable to other diseases.

- *target identification*: Repositional pharmacology involves the identification of potential targets for drug repurposing. This process includes studying the molecular and cellular pathways involved in both the original indication and the target disease. By analyzing the commonalities and differences between these pathways, researchers can identify potential points of intervention and assess the feasibility of repurposing a drug for the new indication.
- *pharmacokinetics and pharmacodynamics*: Repositional pharmacology examines the pharmacokinetic and pharmacodynamic properties of drugs. This includes understanding how a drug is absorbed, distributed, metabolized, and excreted in the body (pharmacokinetics) and how it interacts with its target receptors or biological systems to produce therapeutic effects (pharmacodynamics). Assessing these properties helps determine the appropriate dosing, route of administration, and potential drug-drug interactions when repurposing a drug.
- *safety and tolerability*: Repositional pharmacology considers the safety and tolerability profile of drugs in the context of the new indication. It involves evaluating the known adverse effects, potential risks, and toxicities associated with the drug. By leveraging existing safety data, researchers can determine whether the drug's known safety profile makes it a suitable candidate for repurposing, or if additional safety evaluations or modifications are necessary.
- *preclinical and clinical evaluation*: Repositional pharmacology encompasses preclinical and clinical evaluations of repurposed drugs. Preclinical studies involve in vitro and animal model experiments to assess the drug's efficacy, safety, and potential mechanisms of action in the context of the target disease. Clinical trials are then conducted to validate the repurposing hypothesis, evaluating the drug's efficacy and safety in human subjects.
- *personalized medicine*: Repositional pharmacology can also contribute to personalized medicine approaches by considering individual variations in drug

response. By understanding the pharmacogenomics and pharmacogenetics of a drug, researchers can identify biomarkers or genetic factors that may influence a patient's response to repurposed medications, allowing for tailored treatments and improved therapeutic outcomes.

Overall, repositional pharmacology provides the scientific framework for evaluating the potential of existing drugs in new therapeutic contexts. It integrates knowledge of pharmacological mechanisms, target identification, safety considerations, and clinical evaluations to guide the successful repurposing of drugs, ultimately offering new treatment options and addressing unmet medical needs.

The history of drug repositioning development dates back several decades, with significant milestones and advances along the way [241, 242]. Here is a brief overview of the key moments in the history of drug repositioning:

- *serendipitous discoveries*: Many drug repositioning successes have originated from serendipitous discoveries. Examples include the antimalarial drug quinine being repurposed for the treatment of muscle cramps, and the erectile dysfunction medication sildenafil (Viagra) being repurposed for the treatment of pulmonary arterial hypertension.
- *thalidomide and multiple myeloma*: Thalidomide, a drug originally developed as a sedative and antiemetic, gained attention when it was found to have anti-angiogenic properties. This discovery led to its repurposing as a treatment for multiple myeloma, a type of blood cancer, and demonstrated the potential of repositioning drugs based on their unique pharmacological effects.
- *antidepressants as analgesics*: Tricyclic antidepressants, such as amitriptyline and imipramine, were initially developed for the treatment of depression. However, their analgesic properties were discovered during clinical use, leading to their repurposing as medications for chronic pain management.
- *drug repositioning in HIV/AIDS*: The emergence of HIV/AIDS in the 1980s sparked intense research efforts to find effective treatments. Drug repositioning played a significant role in this context, with antiviral drugs like zidovudine

(AZT), originally developed as an anticancer medication, being repurposed for the treatment of HIV/AIDS.

- *the rise of computational approaches*: With advancements in computational methods and bioinformatics, the ability to analyze large datasets and identify potential drug-disease associations improved significantly. These computational approaches, including data mining, network analysis, and virtual screening, have greatly facilitated the discovery and repurposing of drugs.
- *the repurposing revolution*: In the early 2000s, the concept of drug repositioning gained substantial attention within the pharmaceutical industry and academic research. The realization of the untapped potential of existing drugs, coupled with the challenges and costs of developing new drugs, led to a surge of interest in repurposing as a viable strategy.
- *drug repurposing initiatives*: Various organizations and initiatives have emerged to promote and advance drug repositioning efforts. Examples include the National Institutes of Health (NIH) Chemical Genomics Center's Therapeutics for Rare and Neglected Diseases (TRND) program and the European Union's Innovative Medicines Initiative (IMI) project, both focused on accelerating drug repurposing for unmet medical needs.
- *high-profile repositioning successes*: Several high-profile drug repositioning successes have further highlighted the potential and impact of this approach. For instance, the antihistamine drug loratadine was repurposed as an anticancer agent, and the anti-parasitic drug ivermectin gained attention as a potential treatment for various viral infections.

Some notable examples of successful drug repositioning are presented in review [243]. These examples highlight the potential of drug repositioning to repurpose existing medications for new therapeutic applications, expanding treatment options and improving patient care. It demonstrates the value of exploring alternative uses for established drugs beyond their original indications.

Repurposed drugs have had a transformative impact across various therapeutic areas. In oncology, repurposed drugs have brought about significant breakthroughs.

Existing medications originally developed for other indications have shown remarkable efficacy in treating various types of cancer. By repurposing these drugs, researchers have been able to provide new treatment options and improve outcomes for cancer patients. Beyond oncology, repurposed drugs have made substantial contributions in areas such as infectious diseases, neurological disorders, cardiovascular diseases, autoimmune conditions, and rare diseases. By exploring the potential of existing drugs in novel contexts, researchers have identified new therapeutic uses that extend beyond the drug's original purpose. This approach has not only expanded the treatment options available to patients but has also allowed for the discovery of unexpected mechanisms of action and therapeutic targets. There are some examples of that highlight significant contributions of impact of repurposed drugs in various therapeutic areas:

- *Cancer therapy:* For instance, tamoxifen, originally developed as a selective estrogen receptor modulator (SERM) for breast cancer, has also been repurposed for reducing the risk of breast cancer in high-risk individuals [244]. Additionally, drugs such as thalidomide and lenalidomide, initially developed for other indications, have been successfully repurposed for the treatment of multiple myeloma [245]. Imatinib, initially approved for the treatment of chronic myeloid leukemia (CML), has shown efficacy in other cancers as well. It has been repurposed for the treatment of gastrointestinal stromal tumors (GIST) and certain forms of leukemia, such as Philadelphia chromosome-positive acute lymphoblastic leukemia (Ph+ ALL) [246]. Metformin, commonly used to treat type 2 diabetes, has shown potential as a repurposed drug in cancer therapy. Preclinical and epidemiological studies suggest that metformin may have anticancer effects, particularly in certain types of cancers such as breast, colorectal, and pancreatic cancer [247].

- *Infectious diseases therapy*: For example, anticancer drug initially developed, such as zidovudine [248] have been repurposed for HIV/AIDS. Chloroquine and hydroxychloroquine, originally used for malaria, have been repurposed for the treatment of autoimmune diseases like rheumatoid arthritis and lupus [249]. These drugs gained attention during the COVID-19 pandemic [250]. Dapsone, primarily used in the treatment of leprosy and dermatological conditions, has shown efficacy against certain bacterial and parasitic infections. It has been used in the management of conditions such as *Pneumocystis jirovecii pneumonia* (PCP), toxoplasmosis, and some methicillin-resistant *Staphylococcus aureus* (MRSA) infections [251].

- *Neurological disorders therapy*: For instance, gabapentin, originally developed as an antiepileptic medication, has been repurposed for the treatment of neuropathic pain. It is widely used in the management of neuropathic pain conditions such as postherpetic neuralgia and diabetic neuropathy. Gabapentin is also utilized in the treatment of restless legs syndrome and certain types of migraine [252]. Memantine, initially used for Alzheimer's disease, has also demonstrated benefits in treating other neurological conditions, such as Parkinson's disease and multiple sclerosis [253].

- *Cardiovascular diseases therapy*: Aspirin, originally used for pain relief, has revolutionized the prevention of cardiovascular events by acting as an antiplatelet agent. Drugs like beta-blockers and ACE inhibitors, initially developed for hypertension, have been repurposed for the treatment of heart failure and certain arrhythmias [254].

- *Rare diseases therapy*: For example, nitisinone, originally developed as a herbicide, has been repurposed for the treatment of hereditary tyrosinemia type 1 [255]. Eculizumab, initially approved for paroxysmal nocturnal hemoglobinuria (PNH), has also shown efficacy in treating atypical hemolytic uremic syndrome (aHUS) [256]. Riluzole, approved for the treatment of amyotrophic lateral sclerosis (ALS), has also shown benefits in the treatment of some rare neuromuscular diseases, such as spinal muscular atrophy (SMA) and hereditary spastic paraplegia (HSP). It modulates the release of glutamate, a neurotransmitter involved in neuronal communication [257]. Sirolimus, originally developed as an immunosuppressant for organ transplantation, has been repurposed for the treatment of certain rare genetic disorders, including tuberous sclerosis complex (TSC) and lymphangioleiomyomatosis (LAM). It inhibits a signaling pathway involved in cell growth and proliferation, helping to manage symptoms and slow disease progression [258].

- *Psychiatric disorders therapy*: Antidepressants such as selective serotonin reuptake inhibitors (SSRIs) have been repurposed for other psychiatric disorders, including generalized anxiety disorder and obsessive-compulsive disorder. Lithium, primarily used for bipolar disorder, has also shown benefits in preventing suicidal behavior [259]. Quetiapine, originally approved as an antipsychotic medication, has been repurposed for the treatment of psychiatric conditions beyond schizophrenia and bipolar disorder. It is used in the management of major depressive disorder as an adjunctive treatment and has shown efficacy in reducing depressive symptoms [260]. Bupropion, primarily prescribed as an antidepressant, has been repurposed for the treatment of attention deficit hyperactivity disorder (ADHD) in both children and adults. It helps improve attention, reduce hyperactivity, and manage impulsivity [261].

- *Immunology and autoimmune diseases therapy*: Drugs like methotrexate, originally developed as a chemotherapy agent, have been repurposed for the treatment of autoimmune diseases such as rheumatoid arthritis, psoriasis, and inflammatory bowel disease [262]. Biologics such as infliximab, originally developed for inflammatory bowel disease, have shown efficacy in other autoimmune conditions like rheumatoid arthritis and psoriatic arthritis [263]. Rituximab, originally approved for certain types of lymphoma and leukemia, has been repurposed for the treatment of various autoimmune diseases, including rheumatoid arthritis, systemic lupus erythematosus (SLE), and vasculitis. It targets and depletes B cells, which play a role in autoimmune responses [264]. Azathioprine, originally used as an immunosuppressant in organ transplantation, has been repurposed for the treatment of various autoimmune diseases, including rheumatoid arthritis, inflammatory bowel disease, and systemic lupus erythematosus. It helps suppress the immune response by inhibiting DNA synthesis in rapidly dividing immune cells [265].

- *Respiratory diseases therapy*: For instance, theophylline, initially used for asthma, has been repurposed for the treatment of chronic obstructive pulmonary disease (COPD) [266]. Montelukast, originally developed for allergic rhinitis and asthma, has also been repurposed for exercise-induced bronchoconstriction and eosinophilic esophagitis [267]. Ipratropium, primarily used as a bronchodilator in chronic obstructive pulmonary disease (COPD), has also been repurposed for other respiratory conditions. It is used in the treatment of acute asthma exacerbations and has shown efficacy in reducing excessive respiratory secretions in conditions such as cystic fibrosis [268]. Beclomethasone, a corticosteroid inhaler, has been repurposed for the treatment of various respiratory conditions, including asthma and allergic rhinitis. It helps reduce airway inflammation and control symptoms associated with these conditions [269].

- *Metabolic disorders therapy*: Metformin, a widely used medication for type 2 diabetes, has been explored for potential repurposing in conditions such as polycystic ovary syndrome (PCOS), cancer prevention, and neurodegenerative diseases [247]. The combination of naltrexone and bupropion, originally developed for the treatment of addiction and depression, has been repurposed for the treatment of obesity. This combination medication helps regulate appetite, reduce food cravings, and promote weight loss [270]. Pioglitazone, initially approved for type 2 diabetes, has shown efficacy in the treatment of non-alcoholic fatty liver disease (NAFLD) and non-alcoholic steatohepatitis (NASH). It helps improve insulin sensitivity, reduce liver inflammation, and decrease fat accumulation in the liver [271].

- *Dermatology disorders therapy*: For example, tacrolimus and pimecrolimus, initially approved for organ transplantation and atopic dermatitis, respectively, have been repurposed for other inflammatory skin conditions [272]. Cyclosporine, originally developed as an immunosuppressant for organ transplantation, has been repurposed for the treatment of severe dermatological conditions. It is used in the management of psoriasis, atopic dermatitis, and other immune-mediated skin disorders that are unresponsive to conventional therapies. Cyclosporine helps suppress the immune response and reduce inflammation [273]. Methotrexate, originally developed as a chemotherapy agent, has been repurposed for the treatment of severe psoriasis, psoriatic arthritis, and other autoimmune skin conditions. It helps reduce inflammation, inhibit cell proliferation, and improve symptoms associated with these conditions [262].

- *Gastrointestinal disorders therapy*: Ondansetron, originally developed for chemotherapy-induced nausea and vomiting, has been repurposed for postoperative nausea and vomiting and hyperemesis gravidarum. Proton pump inhibitors (PPIs), primarily used for gastroesophageal reflux disease (GERD), have also been repurposed for the treatment of peptic ulcer disease and *H. pylori* infection [274]. Metoclopramide, originally approved for the treatment of nausea and vomiting, has been repurposed for other gastrointestinal conditions. It is used in the management of gastroparesis, a condition characterized by delayed stomach emptying [275]. Budesonide, primarily used as an inhaler for respiratory conditions, has been repurposed for the treatment of inflammatory bowel disease (IBD). It is used in the management of Crohn's disease and ulcerative colitis, helping to reduce inflammation in the gastrointestinal tract [276].

- *Ophthalmology disorders therapy*: Bevacizumab, originally developed as an anticancer agent, has been repurposed as an off-label treatment for various ocular conditions, including age-related macular degeneration and diabetic retinopathy [277]. Cyclosporine, initially used for organ transplantation, has been repurposed for the treatment of dry eye syndrome. Brimonidine, primarily used as an intraocular pressure-lowering medication for glaucoma, has been repurposed for the treatment of ocular redness. It is available as an over-the-counter eye drop to alleviate redness due to various causes, such as allergies and eye irritation [273]. Carbonic anhydrase inhibitors, such as dorzolamide and brinzolamide, originally developed as glaucoma medications, have been repurposed for the treatment of cystoid macular edema (CME) associated with retinal diseases. They help reduce fluid accumulation and improve macular edema [278].

The field of drug repositioning faces several challenges and holds promising future prospects. One of the major challenges is the identification of suitable candidates for repurposing. Not all drugs have the potential to be successfully repurposed, and careful consideration is required to assess their safety, efficacy, and mechanisms of action in the context of new indications. Additionally, the availability of comprehensive and high-quality data on drug properties, disease biology, and patient populations is crucial for making informed decisions during the repurposing process.

Another challenge lies in the regulatory aspects of repurposed drugs. The regulatory pathways for repurposed drugs may differ from those for novel drugs, and navigating these pathways can present unique hurdles. Adequate communication and collaboration between researchers, pharmaceutical companies, and regulatory agencies are necessary to streamline the regulatory processes and ensure timely access to repurposed therapies.

Furthermore, the financial viability of repurposed drugs is an important consideration. As many repurposed drugs are off-patent or nearing patent expiration, the financial incentives for pharmaceutical companies to invest in further development and clinical trials may be limited. Finding sustainable business models and funding mechanisms for repurposed drugs is essential to incentivize continued research and investment in this field.

Despite these challenges, the future prospects of drug repositioning are promising. Rapid advancements in technology, such as computational modeling, high-throughput screening, and omics technologies, are enhancing our ability to identify new therapeutic applications for existing drugs. These tools enable researchers to analyze large datasets, uncover novel drug-disease connections, and predict drug responses more accurately.

Additionally, the growing emphasis on personalized medicine and precision therapeutics opens up new opportunities for drug repositioning. By considering the genetic and molecular characteristics of individual patients, repurposed drugs can be tailored to specific subpopulations, increasing their effectiveness and reducing adverse effects.

Collaborative efforts among academia, industry, and regulatory agencies are also driving the future of drug repositioning [279]. Initiatives such as public-private partnerships, open-access databases, and data sharing platforms facilitate knowledge exchange, encourage collaboration, and accelerate the discovery of repurposable drugs.

While drug repositioning faces challenges in candidate identification, regulatory pathways, and financial considerations, the future prospects of this field remain promising. Advances in technology, personalized medicine approaches, and collaborative efforts are reshaping the landscape of drug repositioning and opening up new possibilities for repurposed drugs to address unmet medical needs and improve patient outcomes.

Software and various tools play a crucial role in drug repositioning efforts by aiding in data analysis, target identification, and prediction of potential new uses for existing drugs. The field of drug repositioning continues to evolve, and new software tools and approaches are constantly being developed to enhance the efficiency and accuracy of the drug repositioning process.

There are some common applications of software and tools in the field of drug repositioning:

- *data mining and bioinformatics*: Software tools leverage data mining techniques to extract and analyze relevant information from large datasets, including electronic health records, genomics data, chemical databases, and scientific literature. Bioinformatics tools assist in analyzing molecular data, protein structures, and pathways to identify potential drug-disease associations.

- *computational models and machine learning*: Software tools utilize computational models and machine learning algorithms to predict and prioritize potential drug-target interactions, drug-disease associations, and therapeutic outcomes. These tools can integrate multiple data types, such as chemical structures, gene expression profiles, and clinical data, to make predictions and generate hypotheses for drug repositioning.

- *connectivity mapping*: Connectivity mapping tools, such as the Connectivity Map (CMap), utilize gene expression data to identify connections between drugs, genes, and diseases. These tools can help identify drugs that induce similar or opposite gene expression patterns to those observed in specific diseases, suggesting potential new therapeutic uses for existing drugs.

- *network analysis*: Network analysis tools enable the construction and analysis of biological networks, including drug-target networks, protein-protein interaction networks, and disease-related networks. They help identify potential drug targets, assess drug-target relationships, and explore the connectivity between drugs, targets, and diseases.
- *databases and knowledge platforms*: Various databases and knowledge platforms provide comprehensive information on drugs, targets, diseases, and their interactions. Examples include DrugBank, ChEMBL, PubChem, and Open Targets. These resources serve as valuable references and assist in data retrieval, target identification, and exploring drug-disease associations.
- *structural bioinformatics*: Software tools focused on structural bioinformatics analyze the three-dimensional structures of drugs and target proteins. These tools help in understanding drug-target interactions, virtual screening for potential binding sites, and assessing the suitability of existing drugs for repurposing based on their structural compatibility with target proteins.
- *virtual screening and docking*: Virtual screening tools use computational methods to screen large chemical libraries or databases to identify potential drug candidates for specific targets or diseases. Molecular docking tools assess the binding affinity and interaction of drugs with target proteins, aiding in the prediction of drug efficacy and repurposing potential.
- *clinical trial data analysis*: Software tools can assist in the analysis of clinical trial data, exploring the efficacy and safety of drugs in different patient populations and disease indications. They aid in assessing the potential of repurposing existing drugs for new therapeutic uses based on clinical trial outcomes.

There are some examples of software and tools available that can support drug repositioning efforts by helping identify potential new uses for drugs based on their properties and disease information: *TCMSP (Traditional Chinese Medicine Systems Pharmacology Database), DrugCentral, DGIdb (Drug Gene Interaction Database),* *Pharos, Open Targets, DrugBank, STITCH (Search Tool for Interactions of Chemicals), iDrug, DRONet, COVID-19 drug repurposing, PharmMapper, Therapeutic Target Database (TTD), Drug Repurposing Hub, Chemotargets, DrugRep, Vir2Drug*. These tools utilize computational approaches, data mining techniques, and knowledge databases to facilitate the discovery of drug-disease associations.

These databases and platforms offer valuable resources, data, and analytical tools to support researchers in their drug repositioning endeavors. They utilize diverse data sources and algorithms to aid in the drug repositioning process and facilitate the exploration of alternative therapeutic indications for existing medications. They enable the exploration of potential new uses for existing drugs, identification of target-disease associations, and integration of diverse datasets to generate insights for drug repositioning.

Therefore, the repurposing of drugs holds great importance in modern medicine and offers numerous benefits to patients and healthcare providers alike. By exploring new therapeutic applications for existing drugs, repurposing allows for the development of alternative treatment options that can address unmet medical needs, provide cost-effective solutions, and expedite the drug discovery process. Firstly, repurposing drugs can significantly reduce the time, cost, and risks associated with developing new drugs from scratch. Since repurposed drugs have already undergone extensive safety testing and established regulatory pathways, they can be fast-tracked for new indications. This acceleration in drug development enables timely access to potentially life-saving treatments and therapies for patients. Secondly, repurposing drugs can expand the range of treatment options available for various diseases and conditions. By identifying new uses for existing drugs, healthcare professionals can leverage their known mechanisms of action and established safety profiles to address different medical challenges. This approach helps fill therapeutic gaps, especially in rare diseases and conditions where limited treatment options are available.

Furthermore, repurposing drugs contributes to the optimization of healthcare resources and cost-effectiveness. Instead of investing in the lengthy and costly process of developing entirely new drugs, repurposing allows researchers and pharmaceutical companies to focus on exploring the potential of existing compounds. This approach can lead to significant cost savings and efficient use of resources, ultimately benefiting healthcare systems and patients. Looking ahead, the field of drug repurposing holds tremendous promise for further development. Advances in technologies, such as artificial intelligence and big data analytics, are enabling researchers to identify new drug-disease connections more efficiently. By leveraging these tools and expanding our understanding of the underlying molecular mechanisms of diseases, we can unlock even more potential for repurposing drugs.

In conclusion, the repurposing of drugs offers a valuable pathway in the pursuit of improved patient care and therapeutic advancements. Its ability to tap into existing drug libraries, accelerate development timelines, expand treatment options, and optimize resource utilization make it a promising approach for addressing unmet medical needs. The field of drug repurposing holds great potential for shaping the future of medicine and benefiting countless patients worldwide.