

# Case Study



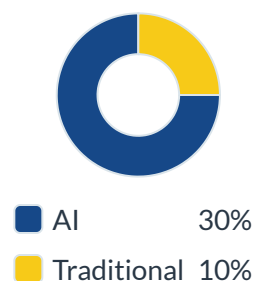
Drug repurposing(DRP)is the identification of new therapeutic use for existing/approved/failed drugs.

## ADVANTAGES OF DRUG REPURPOSING

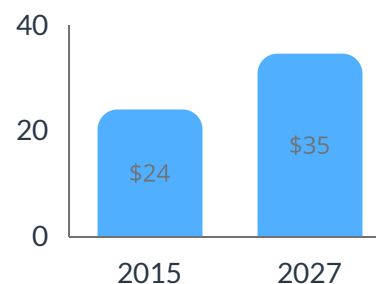
1. Drug repurposing cut down the timeline of identification of potent drugs by nearly 5-7 years.
2. The overall cost for developing a novel drug will be approximately around 2-3 billion, whereas repurposing drugs costs around ~300 million.
3. The approval rate for the repurposed drug is ~30%, 20% more than the traditional approach of identifying new drugs from scratch.
4. In addition to being clinically safe and effective in humans, the important properties like pharmacokinetic property, pharmacodynamics property, and formulation details will be known apriori for the drugs.
5. The market value of the repurposed drug is increasing rapidly and it is expected to reach \$35 billion in 2027 from nearly \$24.4 billion in 2015.

Statistics add that pharmaceutical companies can be benefited from annual revenue of 25% on effective repurposing of drugs.

Approval rate



Market Value of DRP



AI and machine learning approaches are applied to the drug discovery pipeline to speed up and cut down the cost spent on the drug discovery process.

## ADVANTAGES OF AI IN DRUG DISCOVERY

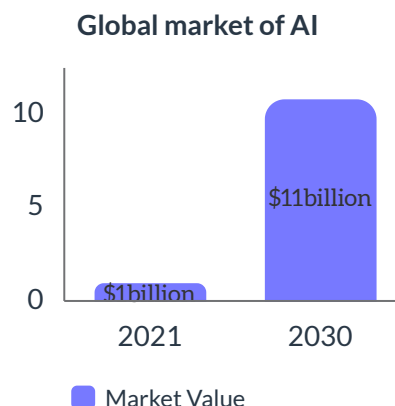
1. In contrast to the traditional approach, AI does not require prior knowledge of the target or the cellular pathway of the disease.
2. It uses complex algorithms to derive knowledge from different data types including omics data, data from the literature, electronic health record, claim data, and many more.
3. Traditional approaches are very well suited for druggable targets whereas the AI approach can also be utilized to identify drugs for undruggable targets.

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4. AI can help pharmaceutical companies to bring down the cost of production of the drug. Statistics show that by 2028, AI can save more than US\$70 billion amount spent on drug discovery.

5. AI with cutting-edge technology can be deployed in almost every stage of drug discovery and development.

Owing to the benefits offered by AI in drug discovery, the global market of AI in drug discovery will reach US\$10.80 billion in 2030 from US\$ 1 billion in 2021, which is increasing at a CAGR of 36%. Hence a majority of pharmaceutical companies are turning to this lucrative technology to increase their share rate.



## MEDVOLT'S AI-DRIVEN DRUG REPURPOSING MODULE

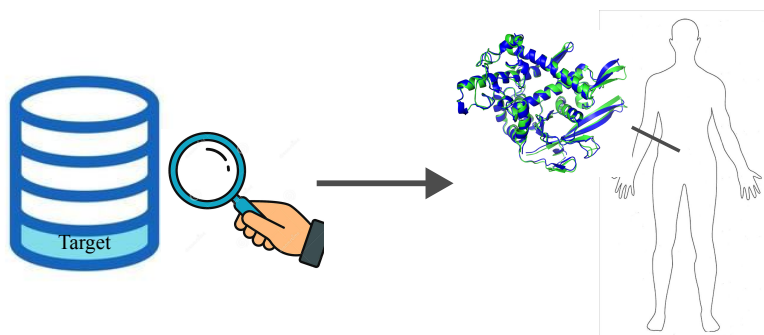
By introducing AI in drug repurposing, we harness the benefits of both techniques in identifying a promising drug for a rare or completely different medical indication.

Our module offers two approaches - Target-based drug repurposing, and compound-based drug repurposing. In target-based drug repurposing, we identify potent drugs for the given target and in compound-based drug repurposing, we identify a novel therapeutic area for the given compound.

We have two separate databases for both target and drug. The data is curated from literature using sophisticated algorithms, and are updated periodically. The target database includes structurally prepared targets and the drug database includes FDA-approved and investigational drugs.

Based on the input, we perform target-based or compound-based filtering to filter out and identify the leads. The leads are identified by ranking them based on docking and protein-ligand interaction fingerprint (PLIF) scores. The PLIF uses machine learning algorithms to identify the interaction of protein and ligand and score them based on the interaction similar to the reference ligand.

We offer state of art molecular dynamics (FEP) for optimizing the lead. The compound-based drug repurposing approach identifies a new therapeutic window for every input drug and the target-based drug repurposing approach identifies safe drugs for the therapeutic target.



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## SALIENT FEATURES

1. User-friendly interface and visualization tools help users to make the right decision in picking the leads.
2. Use of post-docking filter- PLIF and FEP dynamics can help to pick the right drug for the therapeutic condition.
3. AI-driven DRP module can be very well applied to identify drugs for rare diseases.
4. We have skilled SMEs and technical experts to help and give suggestions in every stage of development.
5. Our module is highly customizable. Therefore our customers can avail part of the module services as well.
6. DRP module can be accessed on the cloud and also on premises.
7. In collaboration with CROs, we can take the potent safe drug to the clinic soon.



## Result

Medvolt's AI-driven DRP module with all its advanced state of art techniques and features efficiently identifies a new therapeutic window for all FDA approved and investigational drugs.