

30 alternate indications identified for six shelved compounds

CASE STUDY

Purpose

A large pharma company was looking to expand its portfolio for six shelved assets (four failed in clinical development Phase II & III and two at the preclinical stage) using drug repurposing.

Client



Industry Pharma

Location US



Requirement

The partner was interested in identifying alternate indications for their assets by an integrated strategy. The objective was to combine in silico analysis through Excelra's proprietary platform with validation through wet lab experiments. Indications corroborated through these two independent workflows would be prioritized.

Our approach

The six compounds were analyzed with a comprehensive in silico pipeline. This includes Excelra's proprietary repurposing platform, 'GRIP' to generate a biological rationale for its use in new indications. Further, validation was conducted using a Multi-OMICS approach, conducted in a wet lab to provide a final list of indications per compound

Solution Strategy



In silico analysis





Overview of In-silico Analysis

Excelra's novel and proprietary repurposing platform GRIP (Global Repurposing Integrated Platform) allows for an integrated approach by leveraging the following core components:

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GRIP

The customized Global Repurposing Integrated Database is a compendium of 40+ public & proprietary databases and creates multi-dimensional profiles of biologically relevant entities such as genes, pathways, biomarkers and adverse events



The Holy Trinity

3-way relationships established between drug, disease and target that help understand relevant associations



Algorithms

Customized proprietary algorithms which have been developed internally to mine the drug-target-disease associations from GRID



Analytics & Visualization

In-house analytical capabilities and visualization tools that enable identification of hitherto hidden connections between drugs, disease and targets



Overview of Omics Analysis

Excelra's capabilities in handling OMICs data range across multiple data archetypes. In this engagement, the clients shared drug-treated in vitro & in vivo genomics and metabolomics data for the asset based on the recommendations from the previous in-silico analysis. The multi-OMICs analysis approach used here consisted of analyzing that data to further validate the shortlisted alternate indications that could be recommended to the clients.

The results from the multi-omics analysis were then used to corroborate the in-silico analysis to state the final recommendations, with all the supporting biological rationale in place to validate the final outcomes.



Our contribution

The combined in-silico and multi-omics analyses helped expand the client's portfolio by leveraging data-driven approaches corroborated with wet lab validation, ultimately leading to robust recommendations.

Some key highlights from the outcomes are:

- Alternate indications for the six compounds were identified in silico and validated in vitro/in vivo. One of those compounds progressed to IND filing
- For a compound shelved during preclinical development for the gastrointestinal/ autoimmune disorder was repositioned for Alzheimer's disease
- A compound for which the Target/Mechanism of Action was previously unknown, was repurposed for a new indication using lipidomics data
- For a compound discontinued in clinical development due to hepatotoxicity, an alternate use of diseases requiring topical administration was identified

Our service portfolio

<₀> Data	Data curationFilter out the noise, focus your attentionClinical dataAnalysis-ready data for informed clinical decision-makingSemantic dataRefine your decisions, find your value
Insights	Bioinformatics Illuminating the path to faster discoveries Data science Unlock the power of data Visualization Pictures paint a thousand words
R&D technology	 Product design and development Unlock your potential with data-driven design and development Cloud enablement Optimize your output on the cloud Data engineering Mitigate risks, protect your data, and rationalize your portfolio and processes.

Where data means more

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