excelra

# 30 alternate indications identified for Six shelved compounds

## Objective

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 an integrated drug repurposing approach. Excelra had to propose new indications for these compounds.

## Methodology

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.
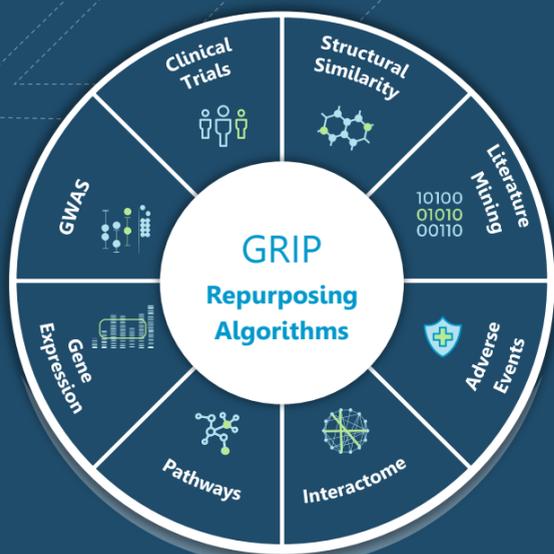
Leveraging integrated *in silico* and multi-OMICS approaches
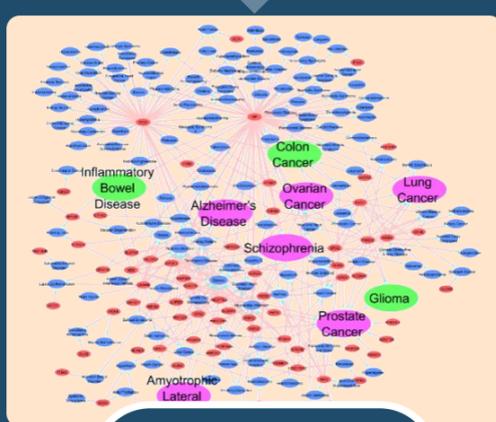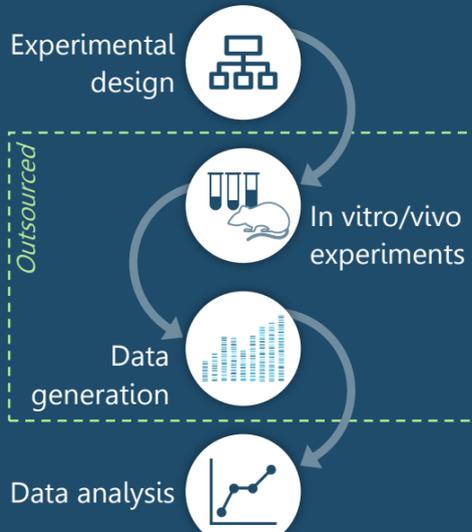
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## *In silico* Approach (GRIP)  |  Multi-OMICS Approach

### Excelra's proprietary databases

**GOSTAR**
(SAR Database with **9+** million compounds, **22million** SAR points)

**GOBIOM**
(Biomarker Database, **120K+** biomarkers across disease areas )

**CTOD**
(Clinical Trail Outcome Database **200+** indications)

**40+** public databases

**GRIP**
**Repurposing Algorithms**

- Clinical Trials
- Structural Similarity
- Literature Mining
- Adverse Events
- Interactome
- Pathways
- Gene Expression
- GWAS

**Analytics Engine & Visualization tools**

Experimental design

*Outsourced*

In vitro/vivo experiments

Data generation

Data analysis

Drug Disease Target network diagram

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## OUTPUT
Top indications for the six compounds based on correlation of both *in silico* and multi-OMICS analysis

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### Results for Compound 1:

| | Glioma | Colon Cancer | Alzheimer's disease | Schizophrenia | Brain Ischemia |
|---|---|---|---|---|---|
| *In silico* | ✓ | ✓ | ✓ | ✓ | |
| Genomics | ✓ | ✓ | ✓ | ✓ | ✓ |
| Metabolomics | ✓ | ✓ | ✓ | ✓ | |

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## Outcomes

- 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 discontinued in clinical development due to hepatotoxicity, an alternate use of diseases requiring topical administration was identified.

- 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.

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At Excelra, we utilize our proprietary technology, GRIP-Global Repurposing Integrated Platform to help our collaborators in their ongoing R&D efforts to build a rich pipeline and provide therapies to patients with pre-clinical and clinical evidence. We have been able to complete 60+ projects in this space providing actionable outcomes that accelerate the drug development process.

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