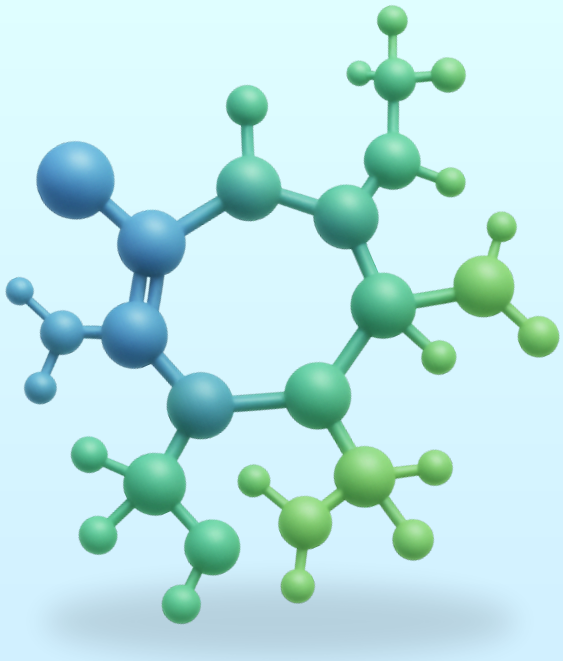
MedGraph Rubie™

AI-Guided Drug Repurposing Engine

Transform existing compounds into new therapeutics using focussed AI, targeted screening and biomedical knowledge graphs

Precision Repurposing | Scientifically Grounded | Clinically Relevant



Scientific Capabilities

Comprehensive drug repurposing powered by cutting-edge AI

Bi-Directional Repurposing

- Predict targets for known compounds
- Screen drugs for new indications
- MOA inference through cross-modality evidence to validate new indications

AI + Physics-driven Screening

- Proprietary Docking + AI-scoring for accurate screening and pose selection
- Optional FEP for ΔG binding affinity (≤2 kcal/mol RMSE)

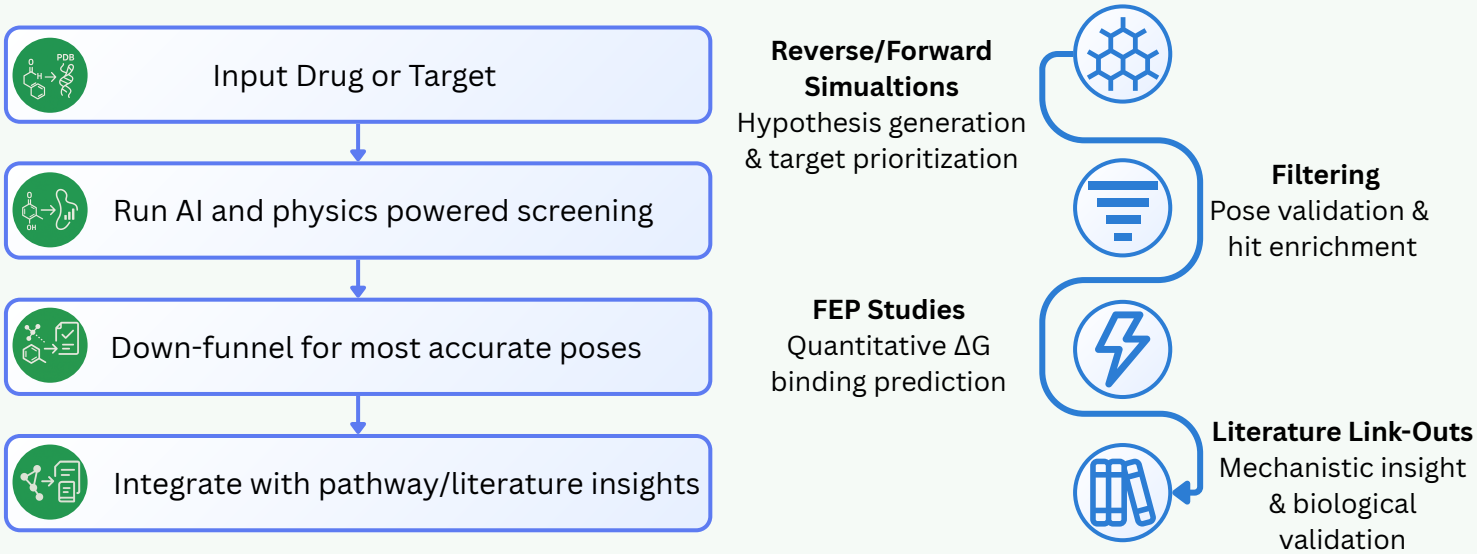
Biomedical Knowledge Graphs

- Integrated knowledge from multiple disparate open and proprietary databases
- AI-driven enrichment with disease-target-drug-gene links and literature context

Ready-to-Screen Libraries

- Approved + Investigational Drugs
- Large on-demand chemical spaces
- Integration with commercial libarries
- Upload custom libraries as needed

Workflow Snapshot



Why Choose MedGraph - Rubie™

Driving Drug Repurposing with Data & AI

100M+
Curated Library

Comprehensive Screening

Rapidly screen multiple large libraries comprehensively with both AI+Physics based methods

Latest
Updates

Knowledge Graph Insights

Leverage structured data stores which are regularly updated to uncover drug repositioning opportunities

10X
Faster

AI + Domain-in-loop

Advanced computational algorithms with domain expert insights ensure precision in lead identification

Greater
Precision

FEP-Enabled Optimization

Free Energy Perturbation (FEP) simulations provide atomic-level accuracy for binding affinity predictions

High
Availability

Scalable & High-Performance

HPC-parallel computing allows efficient large-scale screening for novel drug-target interactions

100%
Secure

Data Privacy & Security

All computations & data transfers are handled with industry-standard data protection

Ideal For

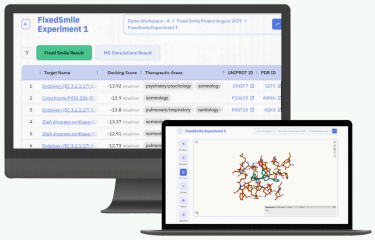
Pharma & Biotech
Reposition shelved/investigational assets

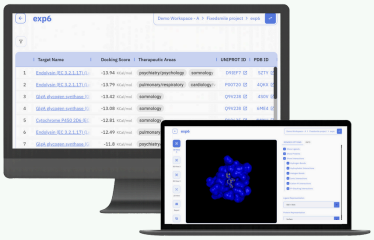
CROs
Rapid indication expansion for partner molecules

Academia & Translational
Hypothesis testing, pathway analysis, polypharmacology

Rare Disease Initiatives
Target discovery where *de novo* design is unfeasible

MedGraph Rubie™





Engagement Model

- Platform Module Licensing
- Insights-as-a-Service
- Knowledge Discovery and Curation
- Co-development

Contact Us

Let's explore how we can support your next discovery efforts

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