

# AI-POWERED CURATION & DISCOVERY SERVICES



## A Deep-Tech company in Pharma R&D

### **Partnering With**

Pharma & Biotech | Startups | Diagnostics | Consulting Firms | CROs | MedTech Companies | Academic Institutions

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### **KNOWLEDGE DISCOVERY**

Harness Medvolt's validated & cutting-edge AI-enabled knowledge discovery solutions and domain expertise to uncover actionable insights for end-to-end R&D



### **MedGraph EDGE**

- Proprietary databases of 10M+ indication-relevant data points
- GenAl + RAG powered engine aggregates, integrates & updates diverse data sources rapidly
- Ontology-based linking for exploring interconnected relationships & causal connections
- Advanced Knowledge Graph to store & uncover hidden insights
- LLM's & RAG to power semantic search, reveal complex pathways & new relationships
- Insights validated by in-house experts

### WORKFLOW



### PROCESS



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### **APPLICATIONS**

- Identification & Prioritization of novel therapeutic targets & biomarkers
- Understanding disease mechanisms & pathways
- Approaches for personalized medicine
- Proprietary database developed over a decade
- Rapid evolution through search engine ingestion
- Customizable to meet client requirements

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### **KNOWLEDGE CURATION SERVICES**

Structured solutions across industry domains with Curated Data-as-a-Service, Al augmentation & Domain expertise to guide strategic decision-making



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# **10M+ Multi-indication Datapoints**

Sourced From



OMICs Data



Publications



Proprietary databases









Grants

#### Patents



Compounds



Customizable to meet client's requirements

### Medvolt's Insilico Services

**Continuous expansion** 

through AI engine

### Small molecule drug discovery workflows with MedGraph<sup>™</sup>

#### HIT ID - FBDD & LBDD

- Generative Al
- Reaction-Enumeration
- Generative Chemistry
- RL Optimization
- Fragment-based methods
- High-throughput Al Screening

#### HIT EXPANSION AND LEAD ID

- MedChem + Advanced MD
- Bioisostere Changes
- Scaffold Hopping
- Functional Group Substitutions



#### LEAD OPTIMIZATION

- Physics-based MD
- SAR Optimization
- Advanced MD FEP
- MedChem Optimization

#### **OTHER CAPABILITIES**

- ML-based ADME-Tox Prediction
- Advanced Molecular Dynamics
- Protein Structure Modelling
- Al-driven Binding Site ID
- Detailed Interaction Studies
- Precision Docking
- Reverse Docking for off-target effects

### Revolutionize your R&D with MedGraph<sup>™</sup>



- **Topaaz**: *De novo* molecule generation with a combination of reaction enumeration & AI-based approaches across structure-based & ligand-based drug discovery paradigms
- **Topaaz MedKush**: Scaffold hopping & functional group substitutions for expanding on hits & advancing to leads
- **Oopal**: Advanced physics-based MD & Free Energy methods across multiple simulation regimes, params & force fields
- **Rubie**: Leverages ligand-based screening & reverse docking, matching drugs & compounds with targets integrated with MedGraph EDGE for knowledge discovery



Multiple rounds of AI-enabled *de novo* fragment-based compound generation & filtering



Deep Learning based optimizations & physics-based advanced molecular dynamics simulations

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