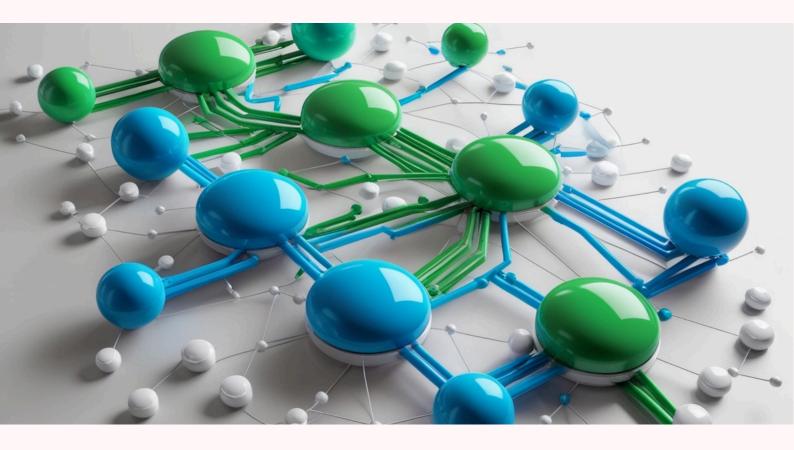


AI-POWERED CURATION & DISCOVERY SERVICES



A Deep-Tech company in Pharma R&D

Partnering With

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

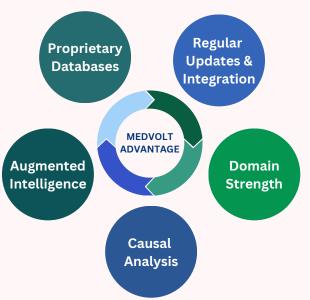
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KNOWLEDGE DISCOVERY

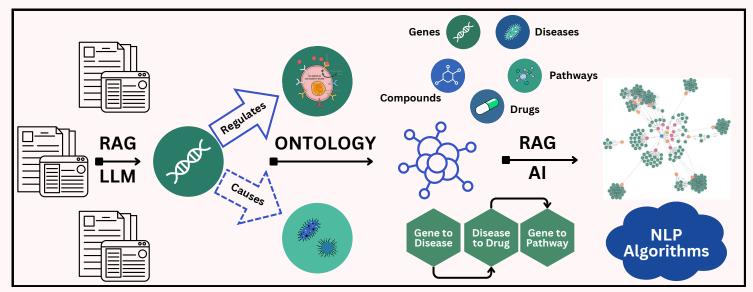
Harness Medvolt's validated & cutting-edge AI-enabled knowledge discovery solutions and domain expertise to uncover actionable insights for end-to-end R&D



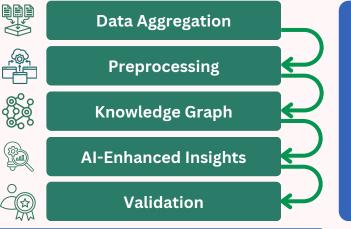
MedGraph EDGE

- 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



Contact Us

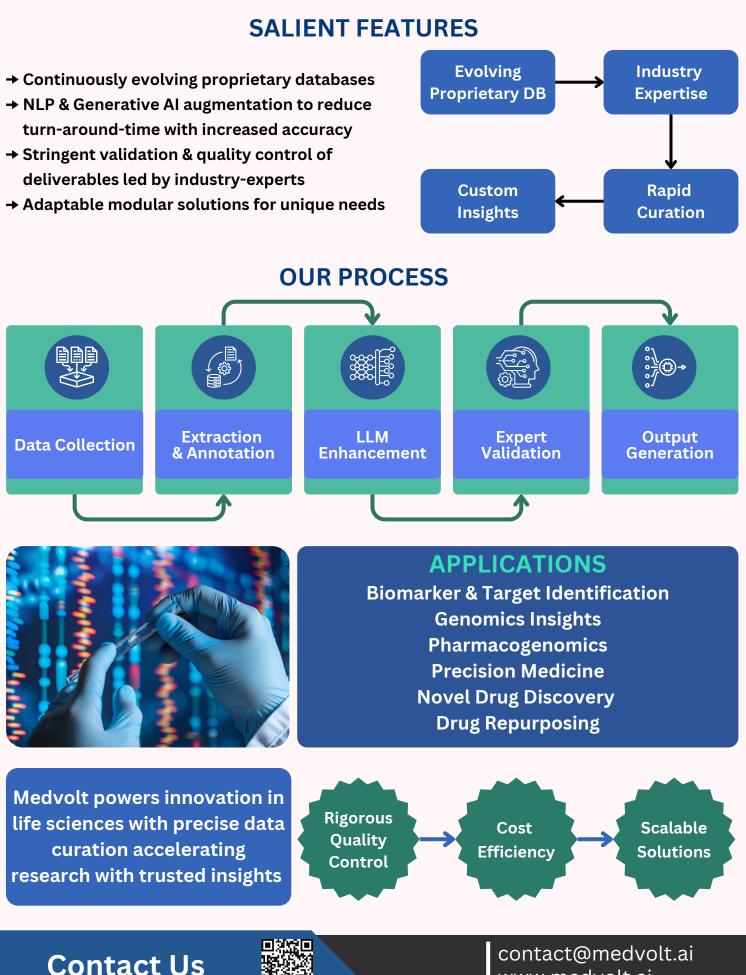
APPLICATIONS

- 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[™]

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[™]



- **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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