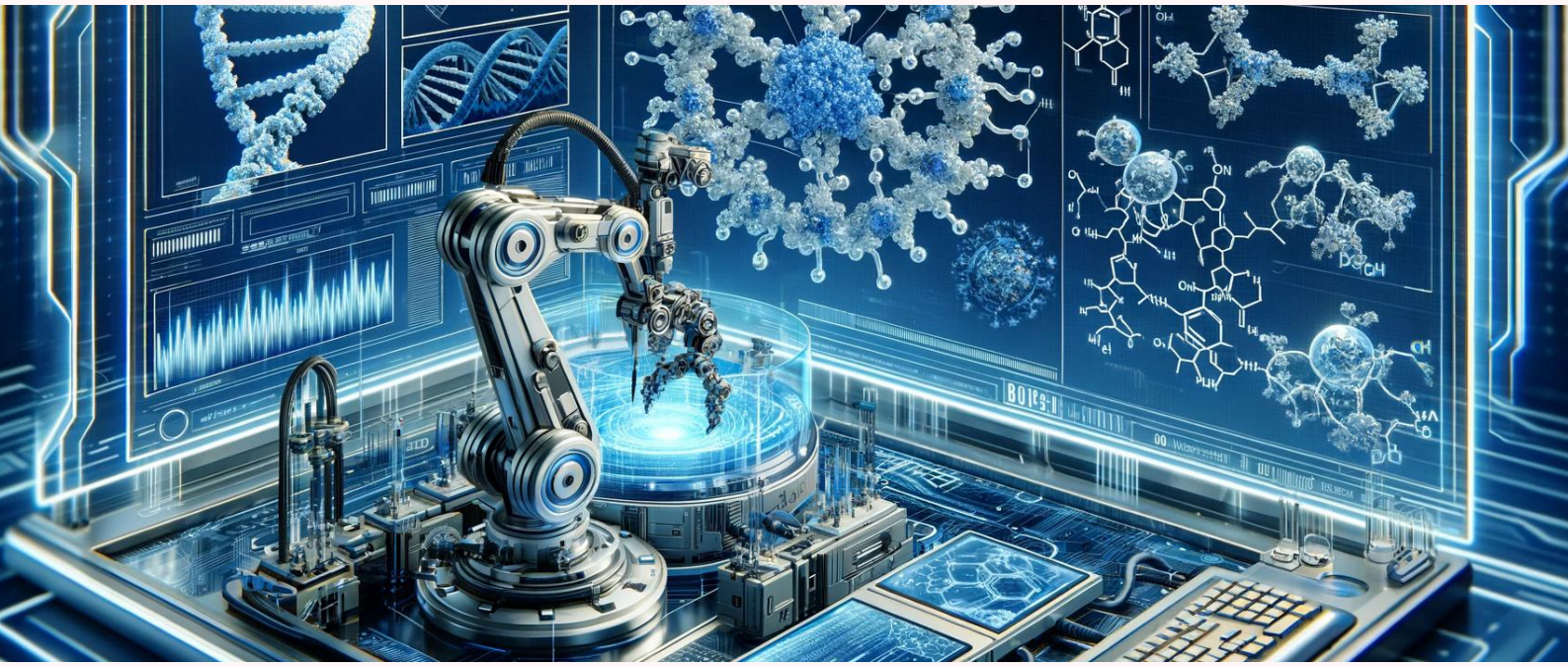
MEDVOLT

DATA-DRIVEN & AI-ACCELERATED DRUG DISCOVERY



A Deep-Tech company in Drug Discovery

Target Identification | Target Prioritization | Drug Design
Biomarker Identification | Knowledge Discovery | Data Curation
Synthetic Chemistry | Experiment Design | Workflow Automation
Customized AI Model Development | Joint Asset Development

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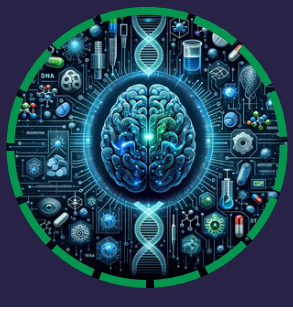
De novo Generation Workflows

- **FBDD** - Generative AI
- **FBDD** - Reaction-Enumeration
- **SBDD** - Generative Chemistry
- **LBDD** - RL Optimization
- **LBDD** - Scaffold Hopping
- **LBDD** - Hit Expansion

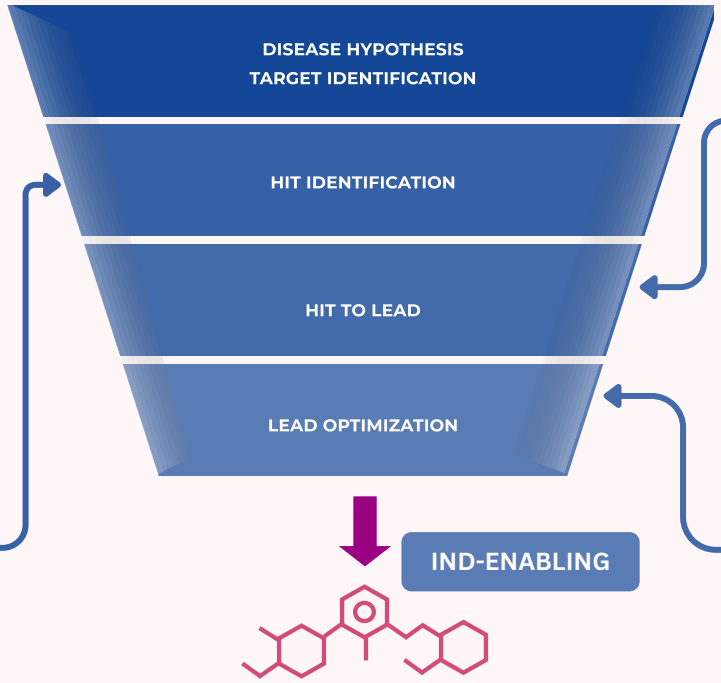


- **Lead ID** - MedChem + Advanced MD
- **Lead ID** - Bioisostere Changes
- **Lead ID** - Physics-based MD
- **Lead Opt** - SAR Optimization
- **Lead Opt** - Advanced MD:FEP-RE
- **Lead Opt** - MedChem Optimization

Four stages of our end-to-end drug discovery pipeline

- Target ID and Scoring
- Binding Pocket ID
- Virtual Screening for Initial Insights
- Experimental and Literature feedback

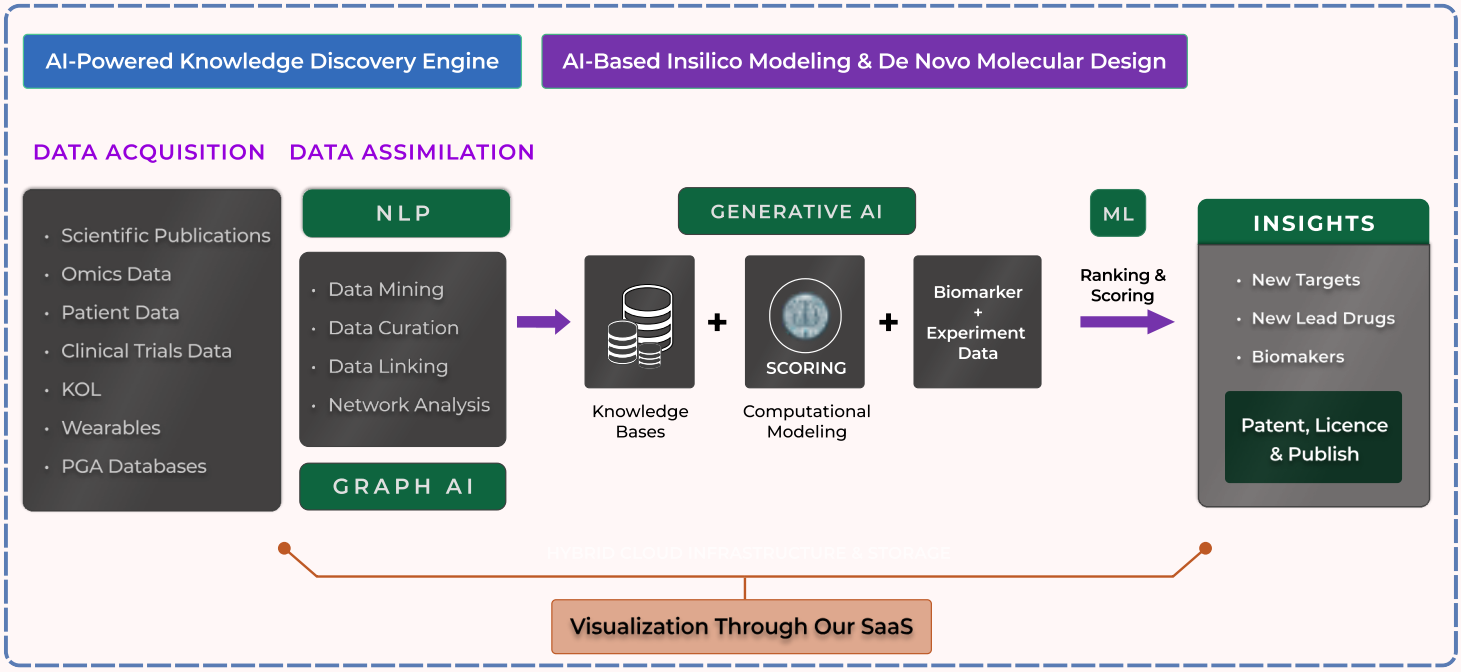
- Generative AI algorithms
- Expansive Chemical Space Exploration
- *De novo* Chemical Space Generation
- Advanced Virtual Screening



- Tailored Chemical Space Exploration
- Accommodating Protein Dynamics
- Advanced MD and Virtual Screening
- Experimental Validation

- Focused Chemical Space for Precision
- MedChem Optimizations
- Integrating Experimental Feedback

Medvolt Platform



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Revolutionize your R&D with MedGraph® for unmatched speed & precision

MedGraph® Topaaz

Small Molecule NCE Module

Submodules:

- Generative AI based de *novo* generation
- MedKush (Hit expansion and Hit-to-Lead)
- cMD + FEP-TI (Thermodynamic Integration)

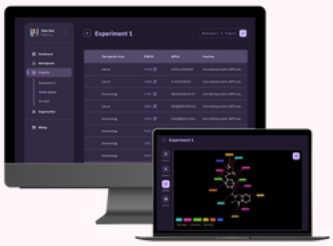
- ***De novo* Generation:** AI and Computational Chemistry methods generate novel hits and offer targetted chemical space exploration
- **MedKush**: Advances hits to leads through scaffold hopping and pharmacophore modeling, integrating QSAR and deep learning for enhanced pharmacokinetics and bioisostere transformations
- **cMD+FEP**: FEP-TI offers a thermodynamic evaluation of ligand affinities and biomolecular conformational dynamics within NCE, supporting the design of bioactively superior molecules

MedGraph® Rubie

Drug Repurposing Module

Submodules:

- Fixed Target | Fixed SMILE
- Knowledge Graph (Knowledge Discovery)
- cMD+FEP (MD + Free Energy Perturbation)



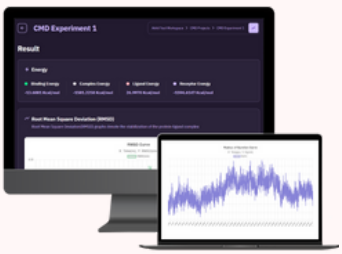
- **Fixed Target | Fixed SMILE**: Leverages ligand-based screening and reverse docking, matching fixed SMILES with novel targets in drug repurposing
- **Knowledge Graph**: Unveils off-target effects and polypharmacology by analyzing multiple data sources in repurposing scenarios
- **cMD+FEP**: Recalibrates interactions of repurposed drugs using QM and MD trajectory analysis and free energy simulations for precise binding efficiency evaluation

MedGraph® Oopal

Advanced MD (Molecular Dynamics) Module

Submodules:

- cMD (Classical Molecule Dynamics)
- Pose Correction MD
- FEP-RE (Free Energy Perturbation-Replica Exchange)



- **cMD**: CMD in Advanced MD leverages enhanced sampling and PMF to delineate the free-energy landscape of drug-receptor dynamics
- **Pose Correction MD**: Prepares molecules for FEP via equilibrium and nonequilibrium MD, ensuring stable drug-receptor interaction complexes
- **FEP Analysis**: Combines unbiased conformational exploration and targeted dynamics, utilizing both unrestrained and restrained FEP for in-depth energetics analysis of ligand modifications' impacts on affinity and specificity

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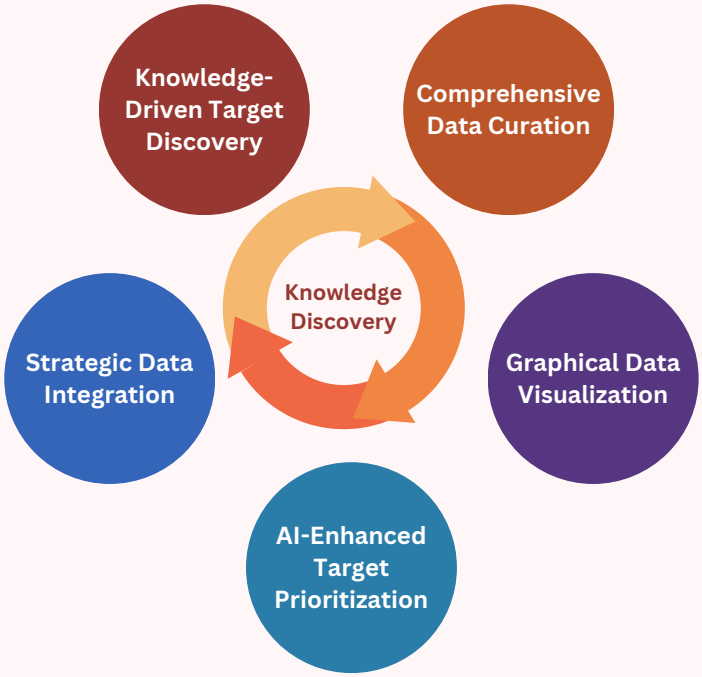
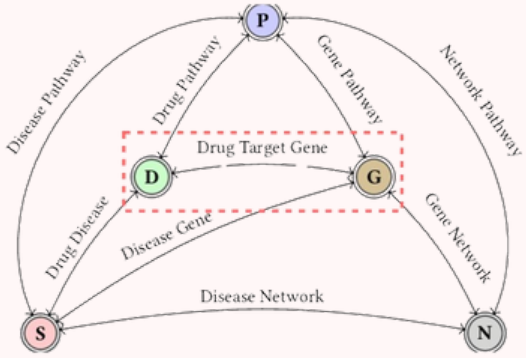
Medvolt's Knowledge Discovery Capabilities

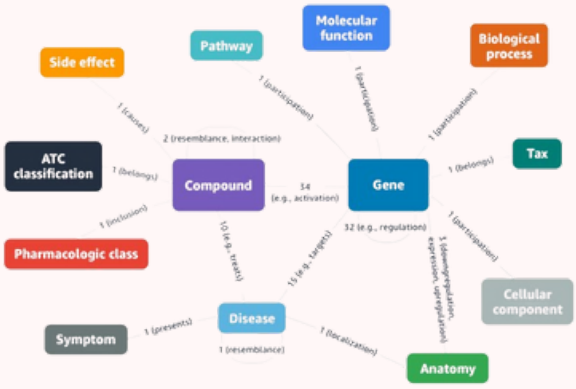
- **Knowledge-Driven Target Discovery**: Identifying therapeutic targets through disease pathway knowledge forms the basis of drug discovery
- **Comprehensive Data Aggregation**: Gathering and synthesizing data from diverse sources using advanced NLP for actionable insights
- **Graphical Data Visualization**: Displaying data as knowledge graphs to reveal the complex relationships between targets, drugs, and diseases
- **AI-Enhanced Target Scoring**: Utilizing generative AI and Large Language Models to accurately uncover disease pathways
- **Strategic Data Integration**: Preprocessing and AI integration to decode complex functional interactions in drug discovery



KD Applications



Medvolt's Knowledge Graph



Partner with Us

Reduce TAT for pre-clinical molecule discovery by ~3x, costs by ~15x and failure-risk by ~25%

Gain an edge with customizable modules for all stages of pre-clinical drug discovery R&D

Enrich your R&D efforts with our robust and proprietary AI-accelerated in silico platform

Leverage on 30+ years of experience across translational biotech

Anchor on gold standard and high-throughput proprietary datasets

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