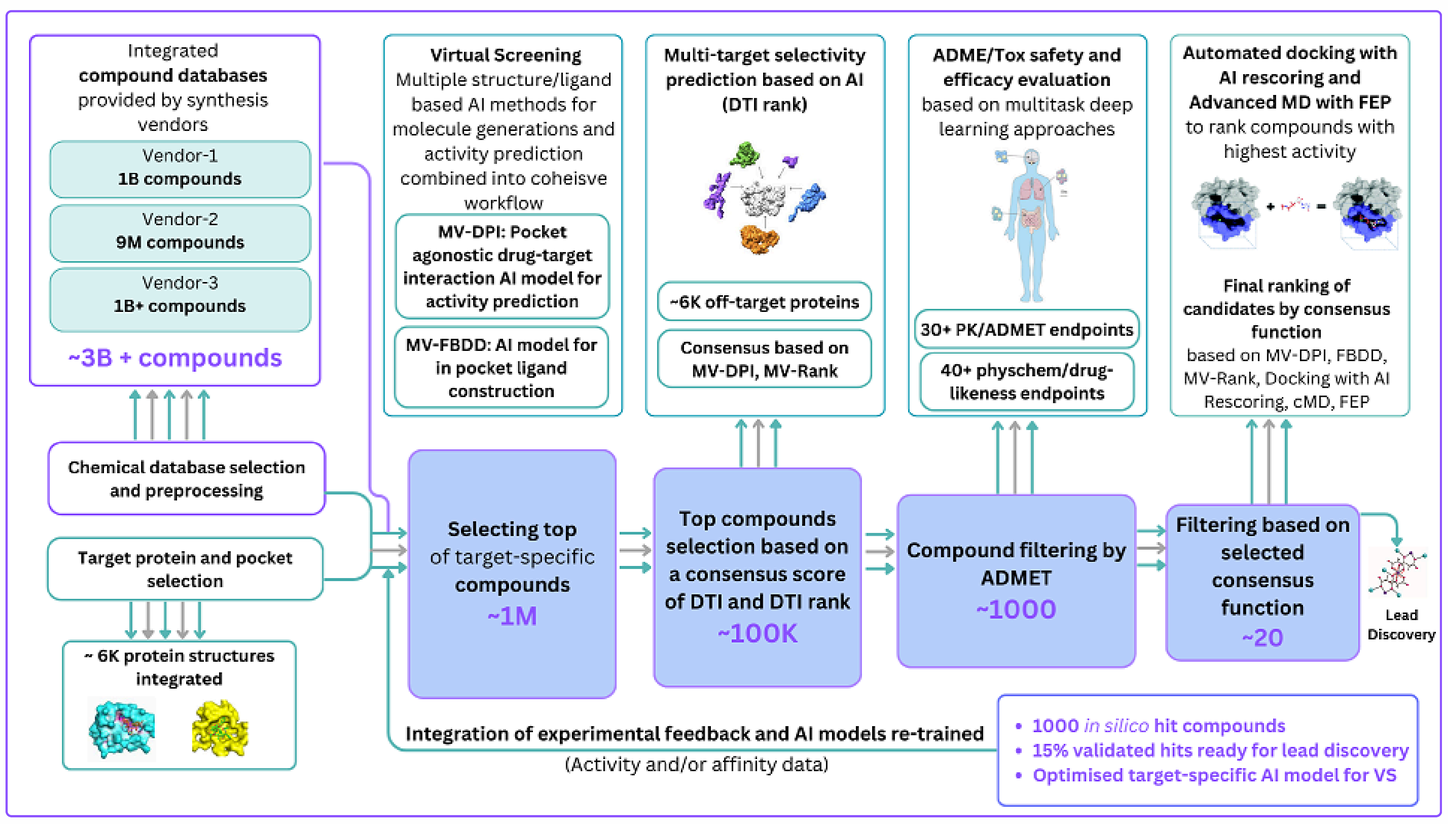
CASE STUDIES: AI & Computational Chemistry for BioPharma R&D

CASE STUDY 2: De-Novo Design via Generative AI and Advanced Molecular Dynamics

- **Context:** Generate *de novo* molecules for high impact targets belonging to Tyrosine Kinase family involved in neuroptosis and inflammatory pathways
- **Objective:** To leverage Medvolt's core platform and Generative AI models to design novel chemical entities (NCEs) targeting the type 3 allosteric site on a key regulatory protein, optimising compounds through an iterative reinforcement learning process and advanced molecular dynamics (MD) simulations for lead optimization

Method + Flow



Allosteric Site Characterization

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Generative AI Based FBDD Module

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RL based optimization loop

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Advanced MD Refinements

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Hit Expansion and Lead Optimization

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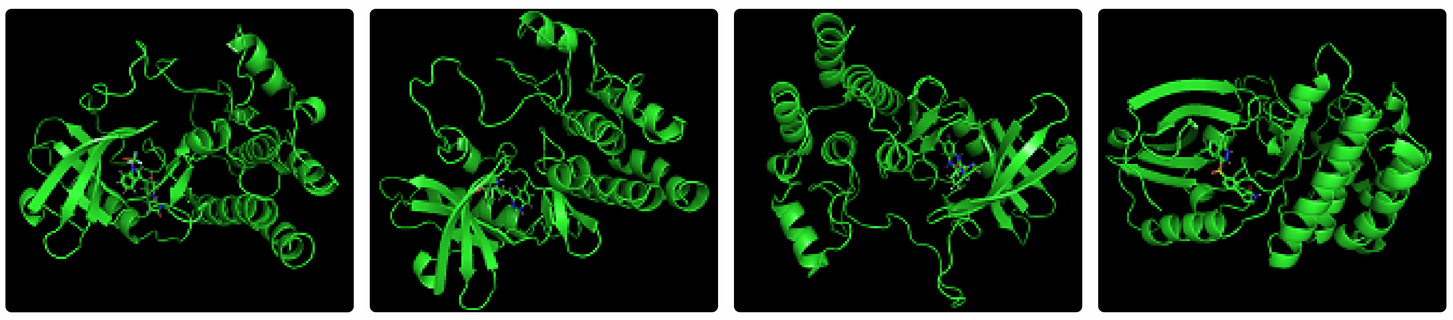
Candidate Selection



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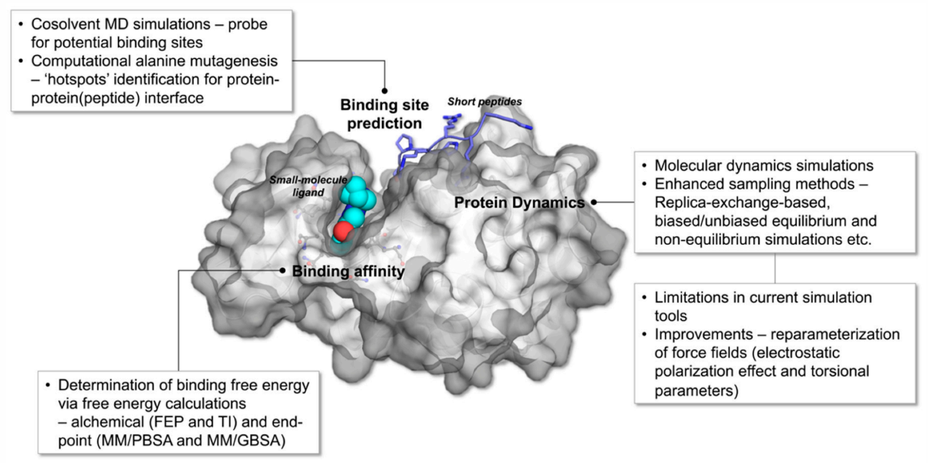

Results

- Created a library of novel fragments targeting allosteric sites with high specificity and stitched them into molecules
- Identified lead entities exhibiting optimal interaction with the regulatory protein's binding site of interest
- Streamlined selection of viable candidates ready for preclinical development pathways

Compounds	FEP Score
Reference Compound	-15.1 kcal/mol
De novo Molecule 1	-14.3 kcal/mol
De novo Molecule 2	-16.5 kcal/mol
De novo Molecule 3	-16.01 kcal/mol