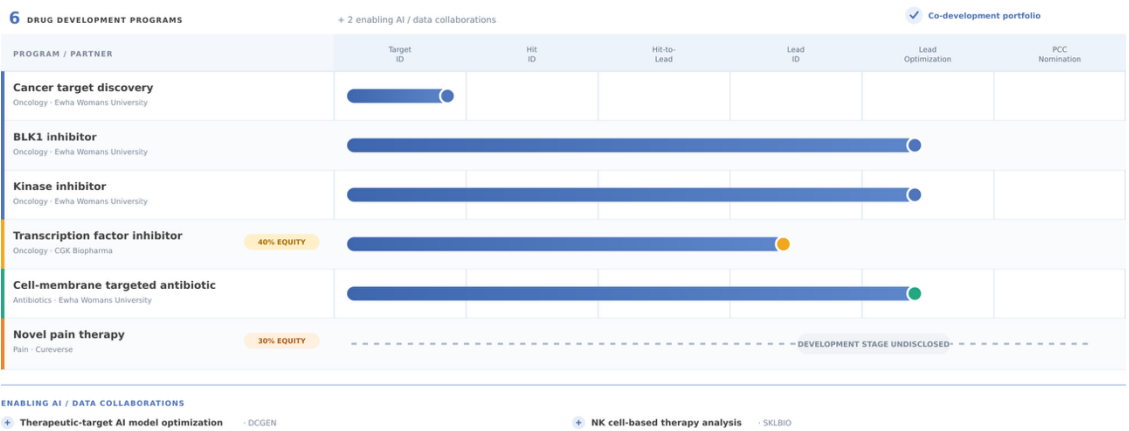
Pipelines



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- Biomarkers in predicting lymph node metastasis. *Scientific Reports*, 2021
- Risk stratification for breast cancer patient. *Cancers*, 2022
- Learning the histone codes with large genomic windows. *Nature Comm*. 2022
- GOAT: biomarker for eosinophilic asthma subtype. *Bioinformatics*, 2023
- DNA deletions occur during DNA repair. *Nature biomed Engineering* 2024
- Multi-layered Knowledge Graph Neural Network Reveals Pathway-level. *CSBJ* 2024
- Increased local DNA methylation disorder. *Nature Comm*. 2025
- MSA-VF: virulence factor prediction. *Scientific Reports*, 2025
- MIL2HET: Single cell-based biomarker discovery. In revision at *BIB*, 2026

Lead Identification/Design/Optimization

Drug Space Identification

- Exploring chemical space for lead identification *CSBJ* 2023
- ChemMining: data-mining with chemical similarity. *CSBJ*, 2023
- DiSCO: molecular conformer optimization. *AAAI*, 2024
- ADME-Drug-Likeness, ISMB, 2025
- Bound.re: predicting drug-likeness, *ICML*, 2025

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- EnsDTI: ensemble DTI prediction. 2024
- Diffusion-based molecular docking. 2024
- ATP binding site prediction. 2024
- MV-CLAM: Multi-View Molecular Interpretation. NeurIPS 2024
- MixingDTA, ISMB, 2025
- CheapNet, ICLR 2025

De novo Drug Design & Optimization

- Generative Modeling to Predict Multiple Suitable Conditions JCIM 2022
- Improved OOD generalization in graph. *CVPR*, 2024
- ChemGen: generative AI models for chemical design. 2024
- RL-Based Molecule Generation, *ICLR2025*
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- M-Frag: Assay-Enriched Fragment Generation. In revision at JCIM, 2026.

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- DRPreter: interpretable drug resp. *Int J Mol Sci*., 2022
- NetGP: drug resp. with target data. *BIB*, 2023
- CSG2A: drug resp. by condition-specific perturbation. *ISMB*, 2024
- DrugPT-Net 2024
- Activity cliff sensitivity into active learning. *ISMB*, 2026

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- SSM: liver toxicity. *iScience* , 2023
- SIDER: side effect. *IEEE JBHI* , 2024
- MDTR: quantifying liver toxicity. Frontiers in Pharmacology2024
- Fate-tox: organ toxicity, *JCI*, 2025

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- PULSAR: in-silico virtual knockout system. 2024
- Inhibitory effects on mushroom, Food sci. and biotech. 2025
- Human immunodeficiency virus-1. eLife 2024
- PONYTA: prioritization of phenotype-related genes. Bioinfo. 2024

Clinical / Market

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- Deep learning survival prediction. ACM-BCB 2023
- Patient survival prediction via transcriptomic and clinical features. BIB. 2025
- Preclinical Drug Response to Patient, *ICLR2025*
- PANDA: Patient-level drug response prediction. ISCBAI, 2026

Drug repurposing

- Exploring Optimal Reaction Conditions. ACS Omega 2022
- DREAMwalk. *Nature Comms.*, 2023
- CAREPath: Semantic Context-Aware Reasoning Paths for Drug Repurposing. BIB, 2026

Drug approval/withdrawal

- Drug withdrawal pred. *IEEE BigComp*, 2022
- ChemAP: drug approval pred. 2024

Artificial Intelligence for **Drug Discovery**

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Broadening
drug discovery
research to
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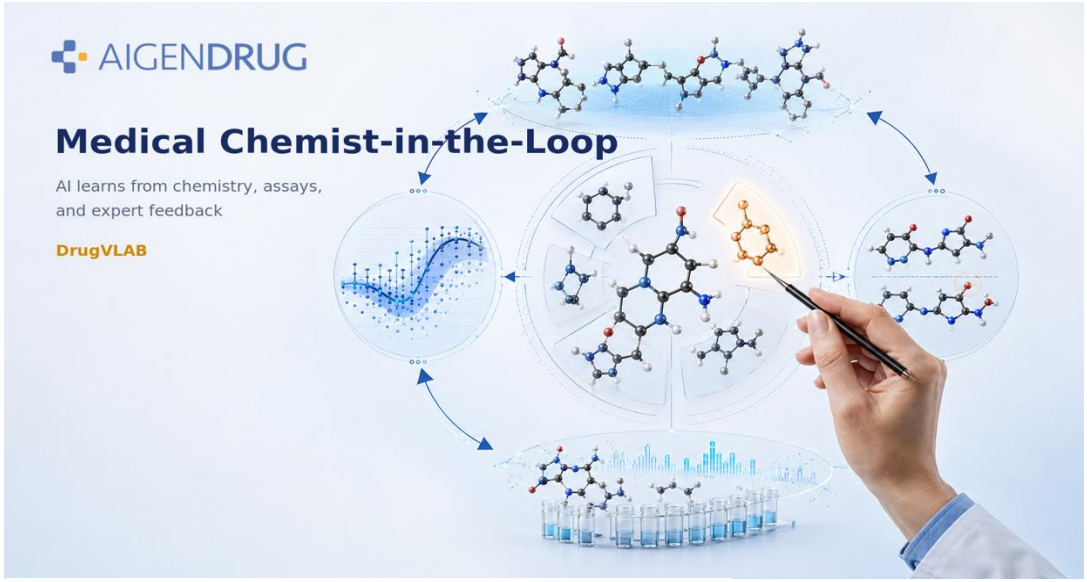
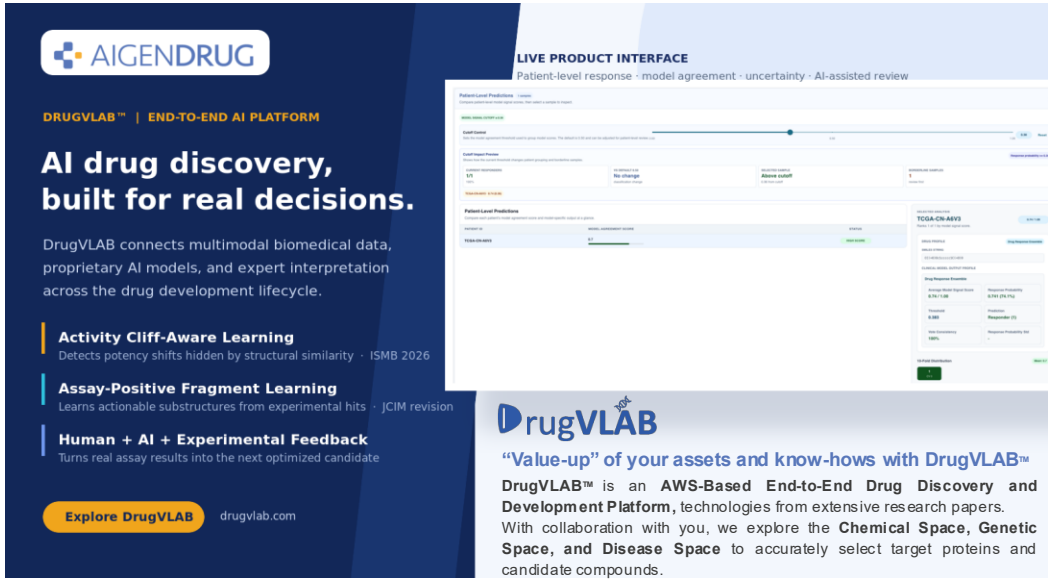
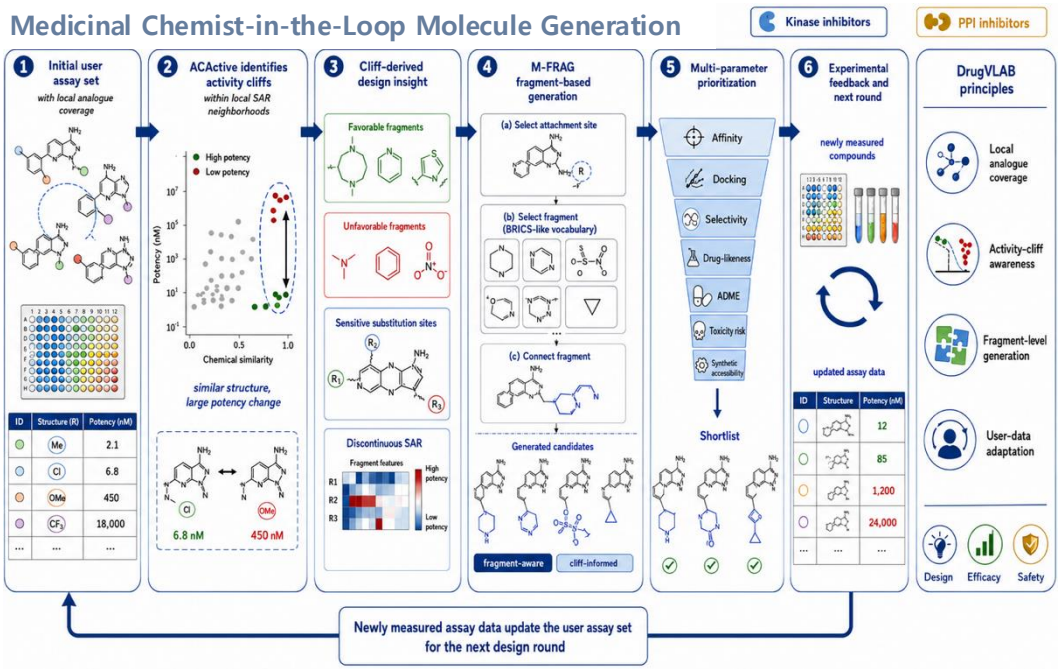
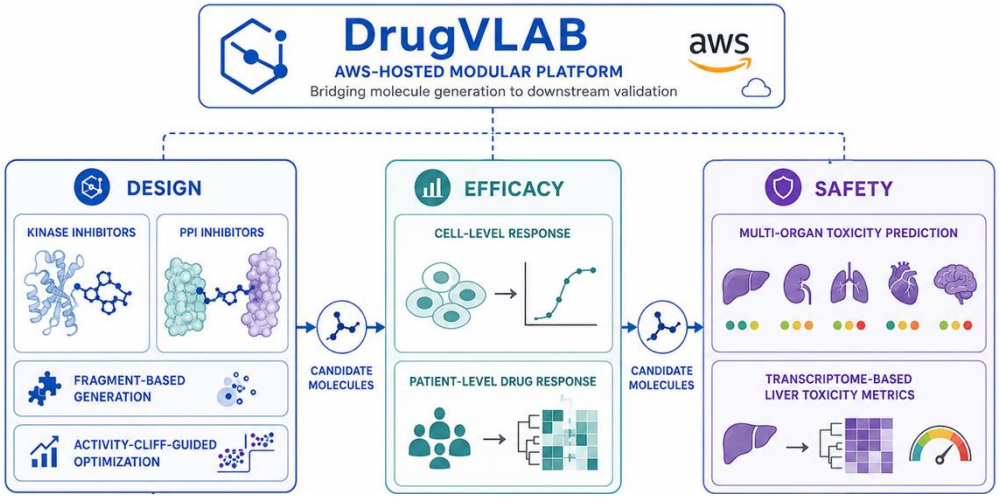
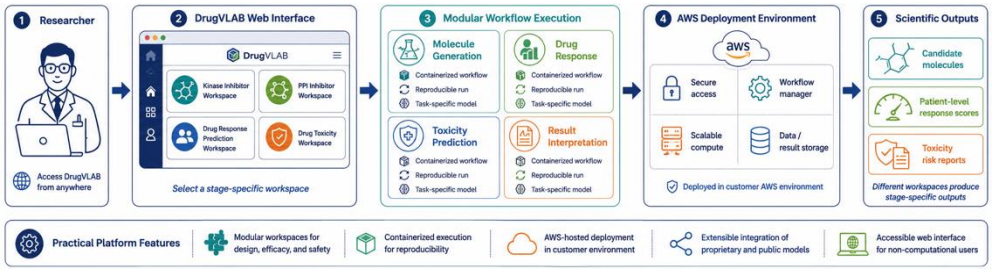








Cloud-Native Modular Execution of DrugVLAB



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