AIDDISON

AI-powered drug discovery SaaS platform combining generative AI, machine learning, and CADD to accelerate hit identification and lead optimization.

https://www.sigmaaldrich.com/US/en/services/software-and-digital-platforms/aiddison-ai-powered-drug-discovery

Overview

AIDDISON™ is a secure, web-based Software-as-a-Service (SaaS) platform developed by MilliporeSigma (the U.S. and Canada Life Science business of Merck KGaA, Darmstadt, Germany) to revolutionize the small molecule drug discovery process. It acts as a comprehensive, 'one-stop-shop' for medicinal chemists by seamlessly integrating Artificial Intelligence (AI), Machine Learning (ML), and advanced 3D Computer-Aided Drug Design (CADD) techniques .

Key Capabilities and Benefits:

AI-Powered Design & Screening: The platform leverages generative AI models (based on REINVENT) to explore unbounded chemical space and design novel small-molecule libraries with optimized structural and ADMET properties . It can virtually screen compounds from a universe of over 60 billion chemical targets, significantly enhancing the efficiency of virtual screening and *in-silico* lead discovery .
Data Advantage: AIDDISON™ is the first commercially available product that includes ML models trained on proprietary, experimentally generated datasets from pharmaceutical R&D, ensuring scientifically valid and reliable predictions . It also incorporates ADME/Tox ML models trained on decades of preclinical data to help reduce development cycles .
Synthesis Integration: A major differentiator is the seamless API integration with **SYNTHIA™ retrosynthesis software** . This connection provides an immediate Synthetic Accessibility (SA) score and proposes synthesis routes, bridging the gap between virtual design and real-world manufacturability .

User Experience: The platform is designed with an intuitive, web-based interface to lower the barrier to entry, enabling less computationally sophisticated medicinal chemists to utilize powerful AI/ML and CADD tools in their daily activities .
Target Users and Use Cases:

Target Users: Medicinal Chemists, Computational Chemists, Drug Designers, and R&D teams in biotech, pharma, and academia .
Use Cases: Hit Identification, Lead Optimization, Scaffold Hopping, Ligand-based and Structure-based Screening, and Synthesis Planning .

Key Features

- Generative AI Molecule Design (De Novo Design)
- Virtual Screening (>60 billion chemical targets)
- Predictive ADME/Tox Modeling
- Synthetic Accessibility Scoring (via SYNTHIA™)
- Ligand-based and Structure-based Drug Design
- Molecular Docking and Shape-based Alignment
- Trained on proprietary pharmaceutical R&D data

Pricing

Model: subscription

Contact MilliporeSigma for a quote. Subscription model designed for small teams, academic users, and enterprise. A free trial is available.

Target Company Size: startup, small, medium, enterprise

Integrations

SYNTHIA™ Retrosynthesis Software, BioSolveIT (FTrees), Cresset (Flare, pyFlare), RDKit, GOSTAR® Databases

Compliance & Certifications

ISO 27001