

# TRANSFORM DRUG DISCOVERY

Drug discovery is complex and requires a multidisciplinary approach. BIOVIA's end-to-end integrated solutions for **Small Molecule Therapeutics Design** help researchers identify high-quality drug molecules faster at reduced costs, while enhancing efficiency and team collaboration. With solutions built over decades of expertise, BIOVIA offers state-of-the-art science powered by physics-based molecular modeling and simulation, AI, machine learning, and lab informatics with the convenience of the **3DEXPERIENCE®** cloud-based platform.



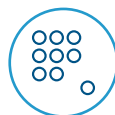
Minimize experimental timelines and R&D costs



Deploy an agile, secure and scalable cloud-based solution with a low total cost of ownership



Facilitate team collaboration and technology transfer to downstream activities



Advance high-quality drug candidates to clinical testing faster



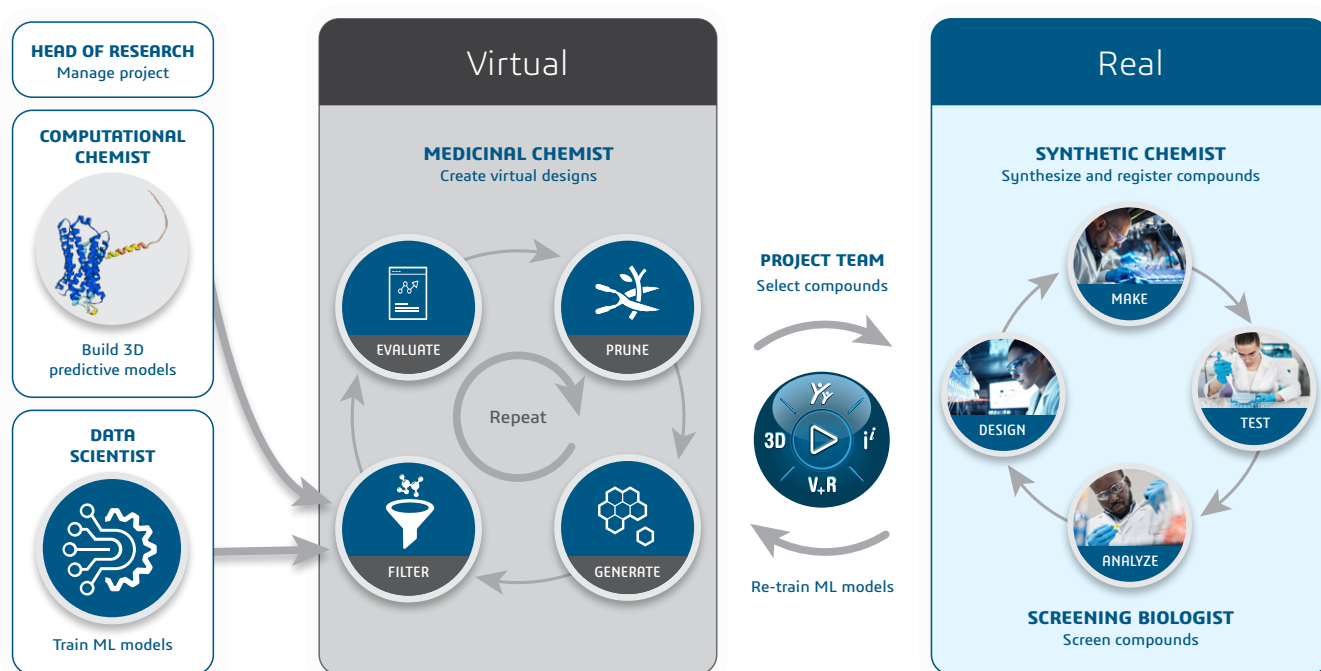
Protect existing intellectual property in the design process

## BENEFITS OF BIOVIA'S COLLABORATIVE SOLUTIONS FOR SMALL MOLECULE THERAPEUTICS DESIGN

- **End-to-End Integration:** Support of entire discovery chain, from virtual target identification and lead optimization to laboratory testing
- **Collaborative Research Environment:** Real-time data access and analysis across multiple teams, in a single platform
- **Predictive Modeling:** Solutions built on over 30 years of expertise in modeling and simulation, scientific informatics, and lab informatics
- **Software-as-a-Service:** Easily deployed with the newest features without the hardware or IT investment
- **Open Architecture:** Ability to incorporate unique custom or 3rd-party models, algorithms, and data sources
- **Data-driven R&D Operations:** Automated and standardized workflows, saving time and resources
- **Data Management and Governance:** Data integrity, security, and traceability throughout the drug discovery lifecycle
- **Flexibility:** Customized workflows adapting to research requirements
- **Scalability:** Solutions accommodating the needs of both small research teams and large pharmaceutical organizations

## BIOVIA MULTIDISCIPLINARY VIRTUAL PLUS REAL SCIENCE

BIOVIA's end-to-end solutions for **Small Molecule Therapeutics Design** support seamless workflows, as multidisciplinary researcher teams move between virtual and real experimentation. Virtual design cycles rapidly generate and optimize new drug candidates before submitting optimized leads to the lab. Real lab data from **Design-Make-Test-Analyze** cycles are used in active learning cycles to retrain Machine Learning models. The Dassault Systèmes **3DEXPERIENCE** platform optimizes the speed and quality of these collaborative activities - all in a single environment.



## A COMPLETE SUITE OF SOLUTIONS ON THE 3DEXPERIENCE PLATFORM

### Machine Learning Workbench

Low-code/No-code application for building and deploying ML models using your **own** proprietary data

### Discovery Studio Simulation

Modeling and simulation suite for building and deploying 3D pharmacophore and docking models

### Generative Therapeutics Design

AI-driven solution for virtual lead optimization that combines machine learning, cheminformatics, and structure-based modeling

### Insight for Research

A scientifically aware, collaborative tool for sharing scientific data and analyzing large datasets

### Scientific Notebook

Electronic lab notebook (ELN) for planning synthetic chemistry experiments and capturing AI-ready data

### Materials Management

A universal system for managing and tracking chemical or biological materials in the lab and for compliance with Environmental Health & Safety (EH&S)

### 3DEXPERIENCE platform

Collaborative multi-disciplinary workspace for real-time sharing, tracking, and managing scientific data and other information related to research projects



For more information, visit  
[www.3ds.com/products/biovia/small-molecule-therapeutics-design](http://www.3ds.com/products/biovia/small-molecule-therapeutics-design)

