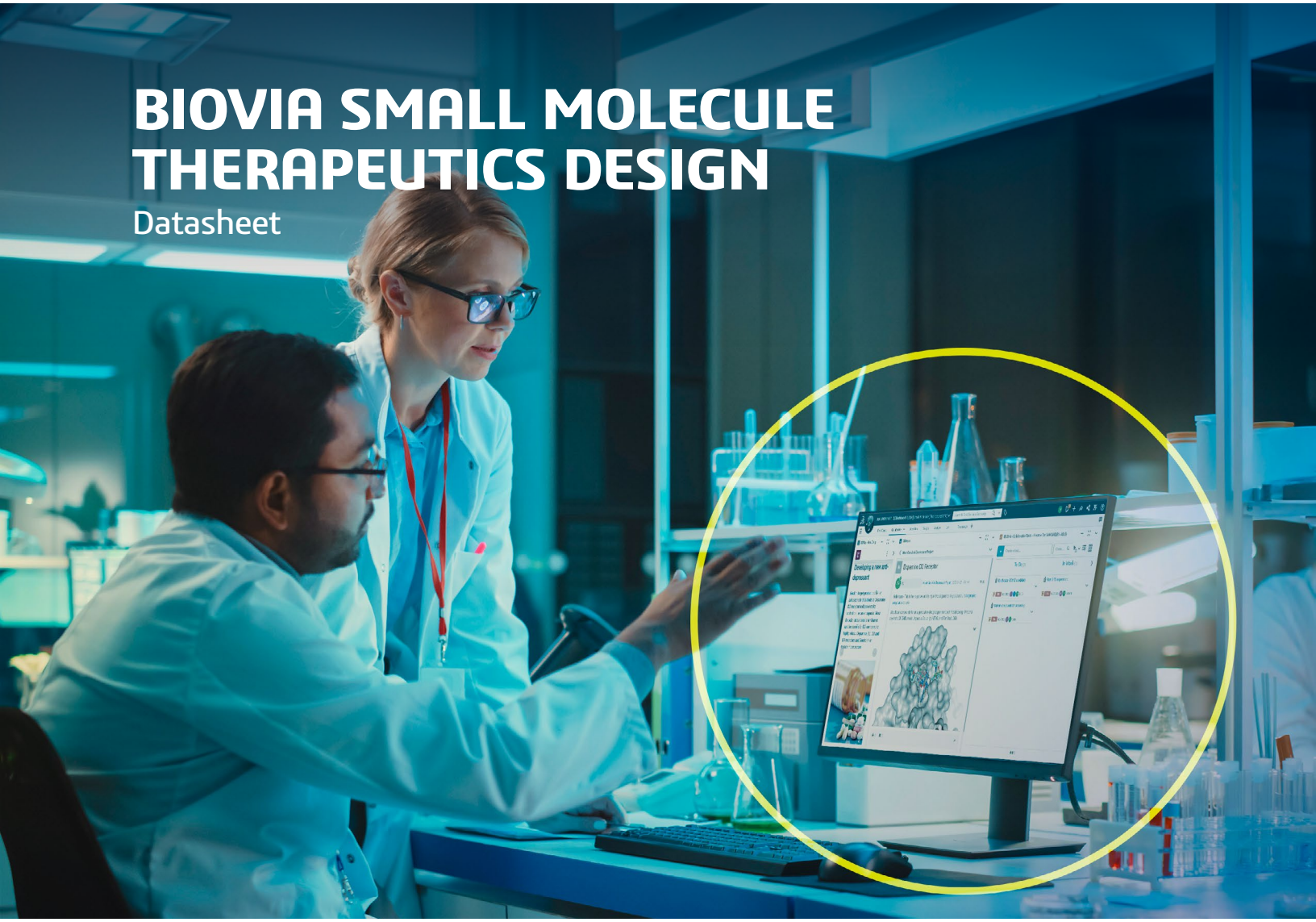
BIOVIA

3DEXPERIENCE®

BIOVIA SMALL MOLECULE THERAPEUTICS DESIGN

Datasheet



ACCELERATE YOUR SMALL MOLECULE DRUG DISCOVERY WITH BIOVIA'S END-TO-END CLOUD-BASED SOLUTIONS

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, AI and machine learning in a single environment, the **3D**EXPERIENCE® platform.

DASSAULT SYSTEMES

COMPLETE SOLUTION FOR SMALL MOLECULE DISCOVERY

BIOVIA has created a collaborative, integrated suite of solutions dedicated for **Small Molecule Therapeutics Design** on the **3D**EXPERIENCE® platform. Together these solutions support drug discovery teams from virtual target identification and lead optimization (**V**) to real lab experimentation (**R**), providing a flexible and scalable approach to drug discovery. Combining the results of virtual generation and evaluation with real world synthesis and testing allows "active learning", improving decision making and collaboration across teams, advancing only the most promising candidates to preclinical testing, while saving money and other resources.

BENEFITS

- **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, on a single platform
- **Advanced Science:** Solutions built on over 30 years of expertise in physics-based modeling and simulation, scientific informatics, and lab informatics enhanced by cutting-edge AI and machine learning technologies
- **Software-as-a-Service:** Easily deployed with the newest features without the hardware or IT investment
- **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
- **Extensibility:** Ability to incorporate unique custom or 3rd-party models, algorithms, and data sources

BIOVIA DISCOVERY STUDIO SIMULATION

BIOVIA Discovery Studio Simulation is a software-as-a-service (SaaS) application on the **3D**EXPERIENCE platform that provide robust and validated modeling and simulation tools to facilitate the design of small molecule therapeutics. Researchers can build pharmacophore or docking models in **Discovery Studio Simulation** and publish these models to be used in **Generative Therapeutics Design** experiments, while capturing virtual experiments in **Scientific Notebook** and registering designed virtual molecules in **Materials Management** – all within the context of role-based experiences on the **3D**EXPERIENCE platform.

Furthermore, **Discovery Studio Simulation** grants users with access to GOLD from the Cambridge Crystallographic Data Centre (CCDC) with no additional license requirement. GOLD is a premier high throughput docking algorithm that has proven success in virtual screening, lead optimization, and identifying the correct binding mode of active molecules.

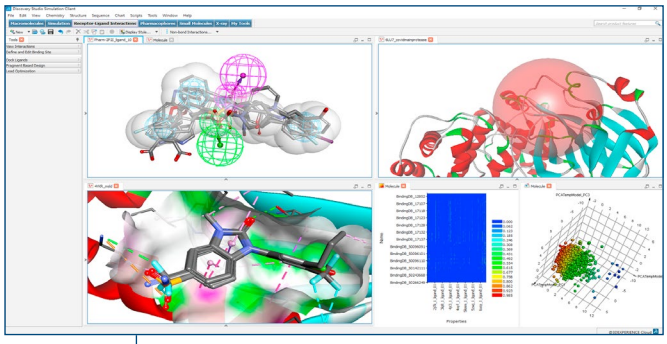


Figure 1: Comprehensive suite of modeling and simulation methods supporting Small Molecular Therapeutics Design in Discovery Studio Simulation

Discovery Studio Simulation also offers protein structure prediction, which utilizes the power of AI with OpenFold/Alphafold. These structures can be used in validated force field-based methods such as Molecular Dynamics (e.g., CHARMm, NAMD). Computational experts can leverage these methods to delve into the biophysical characteristics of solvated macromolecules, gaining insights into mechanisms of action and optimizing essential biomolecular interactions. **Discovery Studio Simulation** also supports the design of small molecules through ligand-enumeration and scaffold-hopping workflows, with additional triaging facilitated by ADMET property calculation and assessments of toxicity and environmental effects.

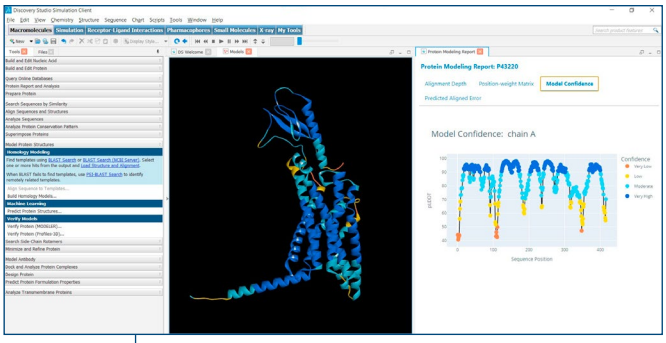


Figure 2: OpenFold/AlphaFold2 models available for structure prediction in addition to long-established, validated homology modeling algorithm MODELER in **Discovery Studio Simulation**

Key Benefits

- Run physics-based modeling and simulation protocols in a High-Performance Cloud Computing environment without the hardware burdens and IT concerns
- Access best-in-class, advanced molecular modeling and simulation tools, including GOLD by CCDC, and AlphaFold2 and OpenFold AI models
- Publish and share docking and pharmacophore models for use in **Generative Therapeutics Design** experiments
- Enhance efficiency and team collaboration with seamless integration to other **3D**EXPERIENCE platform applications such as **Materials Management**

BIOVIA MACHINE LEARNING WORKBENCH

BIOVIA Machine Learning Workbench provides an interactive, user friendly interface for training, validating, and publishing high-quality machine learning models from chemistry data facilitating **Small Molecule Therapeutics Design**.

Using **Machine Learning Workbench**, researchers working on a drug discovery project can build QSAR machine learning models and publish them on the **3D**EXPERIENCE platform to be used by medicinal chemists in **Generative Therapeutics Design**.

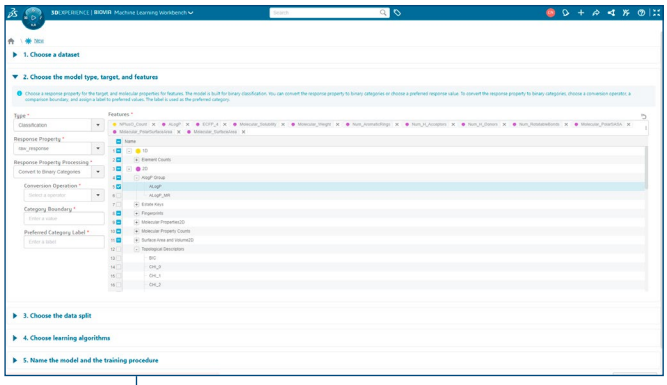


Figure 3: Low-code/No-code QSAR model building with **Machine Learning Workbench**

Key Benefits

- Quickly develop QSAR classification and regression models leveraging all assay data, at any time
- Share and deploy predictive machine learning models easily
- Provide an intuitive user interface to build and manage your models with ease
- Democratize access, fostering innovation across different teams and departments

BIOVIA GENERATIVE THERAPEUTICS DESIGN

BIOVIA Generative Therapeutics Design (GTD) is an AI-driven solution on the **3D**EXPERIENCE platform that automates the virtual creation, testing and selection of novel small molecules.

In the GTD Virtual plus Real (**V+R**) discovery cycle, novel molecules advanced by the virtual generate-filter-evaluate-prune process move to the lab for synthesis and screening. Real world screening results allow the update of predictive models for subsequent cycles. Optimization continues until the desired TPP is met. This iterative **V+R** cycle accelerates lead candidate design with improved quality.

Generative Therapeutics Design guides users through the steps of building machine learning models, defining a target product profile (TPP), executing generative designs including structure generation and filtering, multi-parameter optimization (MPO) based on machine learning and physics-based modeling and simulation methods, and analyzing virtual results together with experimental data (**V+R**).

Figure 4: Improved lead quality with multi-parameter optimization in **Generative Therapeutics Design**

Key Benefits

- Shorten lead optimization phase for drug candidates using AI and machine learning
- Expand the diversity of investigated molecules across the chemical space
- Improve lead quality, with a view to reduce the number of synthesized compounds and experimental assays run per each project
- Deploy an agile, secure, and scalable solution without the hardware burdens and IT concerns
- Enhance efficiency and team collaboration with seamless integration to other **3D**EXPERIENCE platform applications such as **Scientific Notebook** and **Materials Management**

BIOVIA INSIGHT FOR RESEARCH

BIOVIA Insight for Research allows users to visualize, analyze, and browse molecular data proposed by **Generative Therapeutics Design** in detail. Users can compare chemical structures, properties or other custom visualizations and collaborate with team members to make fast, informed decisions on which compounds to synthesize next for testing.

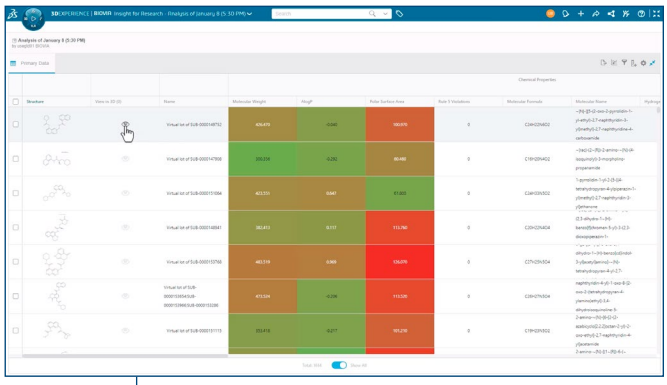


Figure 5: Analyze V+R data to prioritize candidates for synthesis with **Insight for Research**

Key Benefits

- Filter data with substructure search or by choosing the relevant chemical properties
- Visualize data in detail, including 3D chemical structures using Molecular Design
- Analyze results to choose the compounds with overall desirability and best pharmacophore or docking scores
- Collaborate effectively with team members to load, analyze and visualize data, share and comment on results real time
- Work with intuitive web interface that adopts your preferred workflows

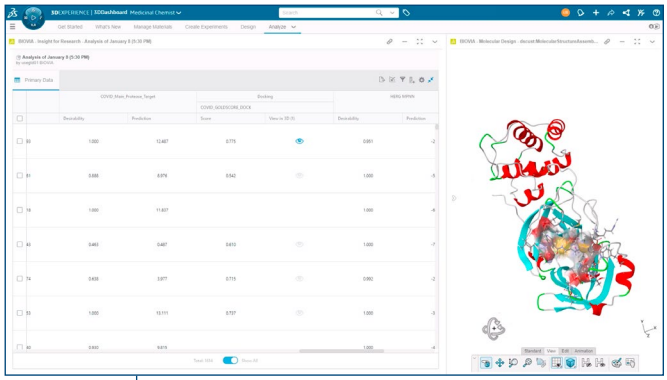


Figure 6: Visualize docking or pharmacophore models and 3D structures with **Molecular Design** integrated **Insight for Research**

BIOVIA SCIENTIFIC NOTEBOOK

BIOVIA Scientific Notebook is a native cloud solution on the **3DEXPERIENCE** platform, prioritizing scientists' needs with a mobile-friendly design, dynamic user-based templates, integrated materials management, and powerful search functions to simplify lab work and documentation efforts.

Scientific Notebook acts as the repository for knowledge, where users can plan experiments, create protocols, and record results, project context and decisions, as well as any other related information.

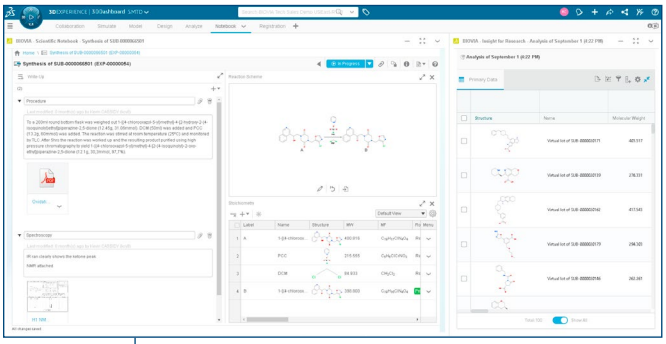


Figure 7: Easy planning and documentation of synthetic chemistry experiments with **Scientific Notebook**

Key Benefits

- Design and modify reaction syntheses and stoichiometry directly
- Add structures through drag-and-drop, with the included structure editor, or by browsing for existing structures in the electronic lab notebook (ELN) library
- Configure the stoichiometry table for custom views with column sorting
- Perform stoichiometry calculations with the built-in calculator
- Add materials from the ELN library, or create them directly within the stoichiometry table
- Save time by leveraging existing knowledge

BIOVIA MATERIALS MANAGEMENT

BIOVIA Materials Management provides scientists with cloud-based UNIVERSAL materials informatics capabilities on the **3DEXPERIENCE** platform. It is built on the rich heritage of BIOVIA registration and material management. Together with **BIOVIA Scientific Intelligence**, **Materials Management** allows drug discovery team members to rapidly capture, identify and locate any chemical or biological material within the system.

BIOVIA Materials Registration supports many steps in **Small Molecule Therapeutics Design**, from the registration of virtual compound ideas to capturing real compounds as lots and determining whether compound ideas may exist already as real compounds in team's inventory. Seamless integration to other **3DEXPERIENCE** applications and services helps improve efficiency and team productivity.

Key Benefits

- Access one universal system for capturing many different types of chemical and biological matter
- Enhance regulatory compliance and inventory management across different teams with standard representation of materials
- Bridge the gap between discovery and downstream activities with seamless integration to **3D**EXPERIENCE platform applications
- Eliminate translation or duplication issues, reducing costs
- Reduce risks with better quality of data and documentation

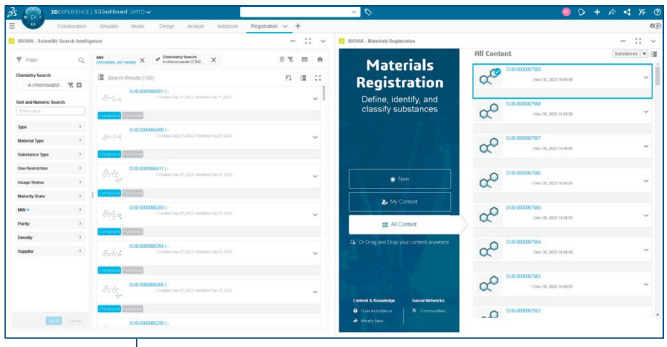


Figure 8: Universal registration of materials with **Materials Management**

A COMPLETE SUITE OF INNOVATIVE SOLUTIONS ON THE 3DEXPERIENCE PLATFORM

BIOVIA's complete suite of solutions support seamless workflows as scientists move between virtual and real experimentation, all in a single environment.

- **BIOVIA Machine Learning Workbench** – Advance drug discovery by building and managing chemistry-based machine learning models that refine your molecular design exploration space
- **BIOVIA Discovery Studio Simulation** – Accelerate drug design with a comprehensive portfolio of validated molecular 3D modeling and simulation tools
- **BIOVIA Generative Therapeutics Design** – Identify high-quality small molecule drug candidates faster with AI and generative design
- **BIOVIA Insight for Research** – Gain insight into your research data to make fast informed decisions while collaborating with internal teams and across networked external organizations
- **BIOVIA Scientific Notebook** – Plan experiments and capture experimental knowledge and context around all of your drug discovery research projects
- **BIOVIA Materials Management** – Capture, identify and locate any chemical or biological material within the system
- **3D**EXPERIENCE **platform** – Collaborate seamlessly across multidisciplinary project teams and among networked partners

LEARN MORE

Our **3D**EXPERIENCE® platform powers our brand applications, serving 12 industries, and provides a rich portfolio of industry solution experiences.

Dassault Systèmes is a catalyst for human progress. We provide business and people with collaborative virtual environments to imagine sustainable innovations. By creating virtual twin experiences of the real world with our **3D**EXPERIENCE platform and applications, our customers can redefine the creation, production and life-cycle-management processes of their offer and thus have a meaningful impact to make the world more sustainable.The beauty of the Experience Economy is that it is a human-centered economy for the benefit of all – consumers, patients and citizens. Dassault Systèmes brings value to more than 300,000 customers of all sizes, in all industries, in more than 150 countries. For more information, visit **www.3ds.com**.

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