BIOVIA

3DEXPERIENCE

FROM MOLECULE TO MEDICINE

Case Studies Leveraging BIOVIA Discovery Studio for Breakthroughs in Biopharma

DASSAULT SYSTEMES

Today's biopharmaceutical landscape is characterized by its complexity, with a pressing demand for drugs that offer improved specificity, safety, and mechanisms of action against increasingly intricate disease profiles.

Addressing these challenges, BIOVIA Discovery Studio presents a robust solution, integrating over 30 years of peer-reviewed research with world-class ***in silico*** techniques such as molecular mechanics, free energy calculations, biotherapeutics developability, and more into a common environment.

This comprehensive suite supports life sciences researchers to explore the nuances of protein chemistry and catalyze discovery of small and large molecule therapeutics from Target ID to Lead Optimization.

The case studies that follow showcase how leading biotech and pharmaceutical companies are utilizing Discovery Studio to address industry challenges, streamline R&D processes, and pioneer new therapies for improved patient outcomes.

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A LEADING CDMO PIONEERS ANTIBODY THERAPEUTICS WITH ADVANCED *IN SILICO* TOOLS

A top global Contract Development and Manufacturing Organization (CDMO), headquartered in China, is dedicated to developing novel antibody therapeutics, aiming to enhance treatment outcomes and accelerate the R&D process affordably.

CHALLENGE

Under pressure to reduce R&D expenses and speed up market entry, the customer sought advanced ***in silico*** tools for protein optimization, analysis, and target screening in order to augment their drug discovery process with more precision.

SOLUTION

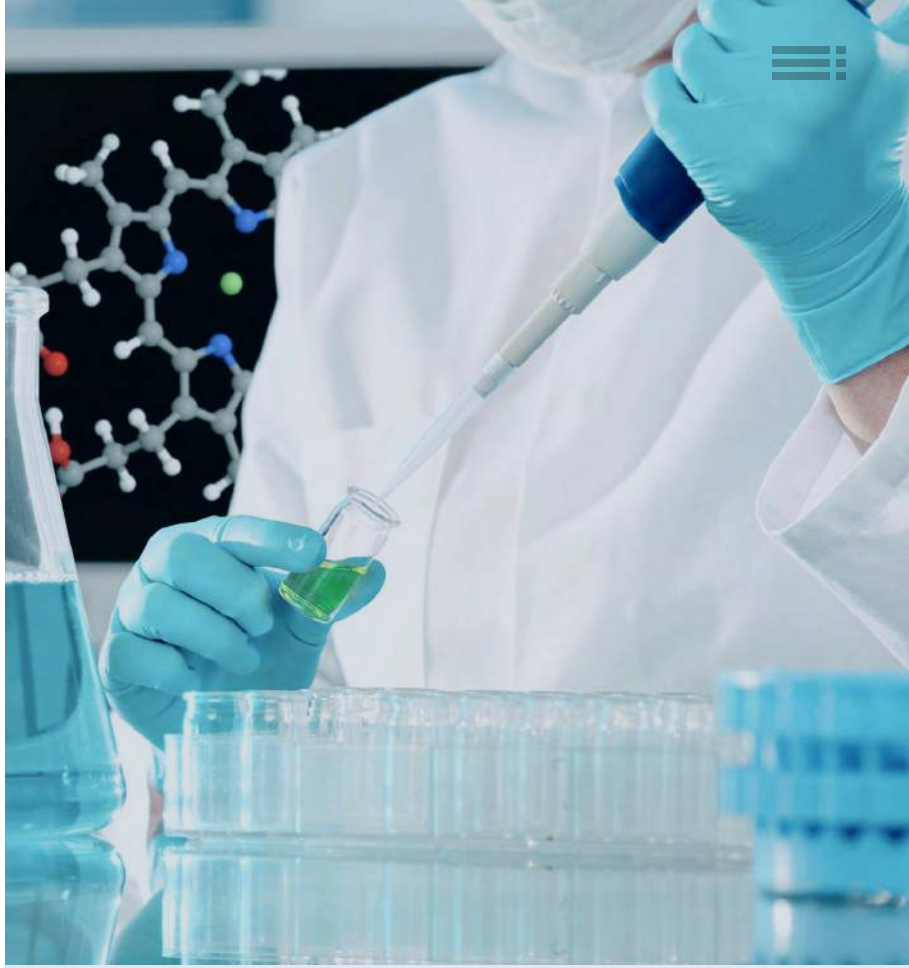
Integrating BIOVIA Discovery Studio, the customer revamped its R&D with ***in silico*** tools for antibody therapeutic development. This suite facilitated protein property calculations, sequence annotation, structure prediction, humanization, and druggability analysis, which in turn enabled the identification and design of candidate compounds and streamlined lab efforts through:

- Comprehensive simulations and analyses focusing on physicochemical characteristics, structural stability, and target affinity.
- Protocols for detailed antibody model quality analysis, enhancing wet lab experiments and decision-making.

OUTCOME

Discovery Studio allowed this CDMO to significantly boost its R&D efficiency in the discovery of novel, effective antibody therapeutics by:

- Accelerating drug development timelines.
- Minimizing risk of failures.
- Providing deeper insights into mechanism of candidate molecules.



"*In silico* tools injected innovative vigor into our drug discovery service process. Through Discovery Studio, we extend our capabilities to analyze proteomic, genomic, and pharmacological data, aiding our clients in identifying new targets and more effective treatment strategies."

A KOREAN BIOTECH STARTUP HARNESSES MOLECULAR MODELING TO ADVANCE IMMUNOTHERAPY RESEARCH

An emerging biotech company based in Korea is dedicated to developing regenerative immunotherapies for patients lacking alternative treatment options. Their mission is to offer new treatments for diseases previously considered untreatable.

CHALLENGE

This biotech company faced challenges in optimizing their novel technology for regenerative immunotherapies. They needed to enhance their insights into molecular interactions within that technology in order to leverage it to its fullest potential.

SOLUTION

To address these challenges, the company applied in vitro and in vivo testing alongside their in-house data for ***in silico*** experiments. They employed BIOVIA Discovery Studio for key tasks:

- Predicting the structure of the Extracellular Vesicle Sorting Motif (ESM) for insights into its interaction with proteins.
- Applying Protein-Protein docking and multimer prediction methods to study intermolecular interactions.

OUTCOME

The use of BIOVIA Discovery Studio has significantly improved the customer's technology by:

- Providing deeper insights into molecular interactions, thus overcoming bottlenecks in their platform technology.
- Maximizing the potential and efficacy of their innovative therapies.

A JAPANESE PHARMA COMPANY ACCELERATES DERMATOLOGICAL INNOVATION THROUGH SIMULATION AND AUTOMATION

A pharmaceutical company based in Japan focuses on the research, development, and production of topical drugs for skin diseases. They aim to bring joy and happiness to patients by improving symptoms, allowing them to resume normal lives.

CHALLENGE

Faced with the industry-wide challenge of reducing R&D time and costs, the customer looked for methods to validate their hypotheses ***in silico***, streamlining the path to market for new treatments.

SOLUTION

Leveraging the capabilities of BIOVIA Discovery Studio, the customer embarked on an in-depth exploration of their drug candidates through:

- Molecular modeling and simulation for detailed insights into the drugs' mechanisms of action, aiding in both target identification and the improvement of candidate compounds for lead optimization.
- Utilization of BIOVIA Pipeline Pilot to enhance efficiency through automation, creating and deploying custom workflows, and integrating a variety of data sources, databases, and third-party or in-house tools.

OUTCOME

By integrating Discovery Studio and Pipeline Pilot into their workflow, they:

- Achieved significant reductions in both the time and cost associated with bringing new products to market.
- Drove the scientific process from the ground up, from identifying targets to optimizing lead compounds.
- Improved productivity on an individual level and fostered better collaboration across teams.

A GLOBAL BIOTECH COMPANY SHAPING CANCER TREATMENT WITH PREDICTIVE ANTIBODY DESIGN

A clinical-stage biotech company located in France specializing in oncology aims to improve patient outcomes by developing therapeutic antibodies that harness the immune system to fight against cancers.

CHALLENGE

The company was in search of an ***in silico*** method capable of characterizing and optimizing the most promising antibody candidates, as well as enhancing target binding to improve the efficacy of their therapeutics.

SOLUTION

Employing BIOVIA Discovery Studio, the company identified the best variants with the highest affinity. A key part of their strategy involved using the humanization protocol to reduce the immunogenicity of their candidate antibody therapeutics.

OUTCOME

BIOVIA Discovery Studio enabled the company to:

- Virtually predict and design multispecific antibodies targeting both immune and tumor cells.
- Reduce the need for physical experiments, saving time and resources.
- Develop antibodies with lower immunogenicity, enhancing safety and effectiveness.
- Improve patient outcomes through superior antibody development.

"With Discovery Studio's predictive capabilities, we are performing less experiments, saving significant time and costs. We also achieve better results and develop better antibodies for patients."

FROM MOLECULE TO MEDICINE

The pharmaceutical industry has experienced a boom of innovation over the past two decades. The leaders in the Life Sciences industry are partnering with BIOVIA, a Dassault Systèmes brand, to accelerate their drug discovery using BIOVIA Discovery Studio. Discovery Studio is uniquely positioned as the most comprehensive 3D modeling and simulation application for the Life Sciences discovery research.

It offers a wide range of powerful tools that enable computational chemists and computational structural biologists to engineer stable and optimized novel biotherapeutics and small molecule drugs with desired safety profiles.

For more information, visit **www.3ds.com/products/biovia/discovery-studio.**

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