

DRIVING EFFICIENCY AND SAFETY IN ANTIBODY DISCOVERY WITH *IN SILICO* SOLUTIONS

Use Case



Challenge:

Optimizing bispecific antibody candidates and reducing immunogenicity with traditional methods proved time- and resource-intensive.

Solution:

The company adopted BIOVIA Biotherapeutics Design solutions for *in silico* modeling and simulation to optimize candidates and reduce immunogenicity.

Results:

Enhanced candidate quality, reduced late-stage failures, and accelerated development timelines with significant resource savings.

THE CUSTOMER A GLOBAL BIOTHERAPEUTICS INNOVATOR

A clinical-stage biotechnology company in China is dedicated to improving cancer treatment outcomes through innovative therapeutic antibodies that harness the immune system.

Focusing on oncology, the company collaborates with leading global biopharmaceutical firms to accelerate R&D and introduce next-generation antibody-based treatments more rapidly.

With expertise in antibody development and access to advanced technologies, the company drives significant advancements in cancer care. A dedicated team of researchers keeps them at the forefront of innovation, continuously improving outcomes for cancer patients.

CHALLENGE OVERCOMING ANTIBODY DISCOVERY BOTTLENECKS

The company develops bispecific immune cell engagers that target and destroy tumor cells. However, optimizing and validating these candidates posed significant hurdles. Traditional screening methods were labor- and resource-intensive, requiring lengthy timelines. Additionally, reducing immunogenicity through humanization protocols added further complexity, slowing development and driving up costs.

To address these hurdles, the company needed an advanced *in silico* solution that leverages computational modeling and simulation to identify high-quality candidates with optimal efficacy and safety. Specifically, they sought a platform that could:

- Predict binding interactions.
- Optimize antibody variants.
- Evaluate immunogenicity risks during early development.

By adopting such a solution, they aimed to streamline their discovery, improve candidate quality, and accelerate timelines while reducing the costs.

SOLUTION

IN SILICO MODELING AND SIMULATION WITH BIOVIA BIOTHERAPEUTICS DESIGN SOLUTIONS

BIOVIA's comprehensive Biotherapeutics Design solutions empower researchers to accelerate discovery workflows and reduce time-to-market. These solutions identify the best biotherapeutic candidates while meeting regulatory, business, and market requirements.

With BIOVIA's platform, computational structural biologists can follow a strong and reliable workflow for designing antibody-based therapies. The benefits include:

- Perform protein-protein docking with ZDOCK
- Simulate protein structure flexibility and analyze molecular interactions.
- Predict formulation properties such as aggregation, viscosity, solubility, and developability.
- Perform humanization to reduce immunogenicity and improve safety profiles.

Powered by the **3DEXPERIENCE®** cloud, BIOVIA solutions provide scalable, high-performance computing for complex modeling and simulations. Researchers can also register virtual designs and record experiment details, enabling seamless workflow integration.

RESULTS ADVANCING BIOLOGICS DISCOVERY WITH IN SILICO INNOVATION

Since adopting BIOVIA's discovery platform, the company streamlined workflows to design bispecific antibodies targeting immune and tumor cells.

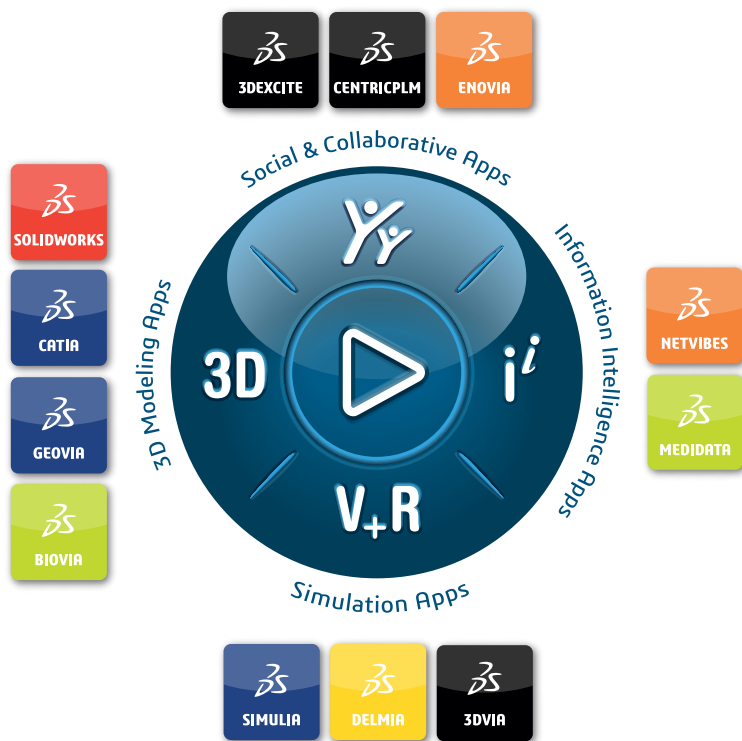
Key outcomes include:

- **Enhanced Efficiency:** *In silico* design reduced physical experiments, saving time and resources.
- **Improved Safety:** Early identification of immunogenicity risks led to safer bispecifics without compromising efficacy.
- **Accelerated Timelines:** Virtual predictions identify poor candidates earlier, reducing late-stage failures and improving developability.

By addressing candidate optimization challenges early, the company delivers next-generation biotherapeutics faster and more efficiently, improving outcomes for cancer patients.

"By using BIOVIA Biotherapeutics Design portfolio, we're achieving highly predictable results that are quickly and easily obtained. This reduces the number of samples we need to produce and test experimentally, saving us both time and costs. Ultimately, we get better outcomes and more effective antibodies for our patients."

— R&D Head, Clinical-Stage Biotechnology Company



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