BIOVIA

3DEXPERIENCE®

PREDICTING EXCIPIENT PROPERTIES WITH BIOVIA MATERIALS STUDIO

HOW SANOFI STREAMLINED DRUG FORMULATION DESIGN

Use Case

DASSAULT SYSTEMES

Challenge:

Autoxidation testing being a costly bottleneck for Pharmaceutical Development.

Solution:

BIOVIA Materials Studio to better understand and predict formulation properties.

Results:

- Shortened drug development cycle by 6 months
- Improved risk assessment for target drug compounds and potential formulations
- Reduced spend on materials and disposables with in silico experimentation
  two projects

THE CUSTOMER
A GLOBAL BIOTHERAPEUTICS INNOVATOR

With a broad portfolio of products covering human vaccines, rare diseases, multiple sclerosis, oncology, immunology, infectious diseases, diabetes, cardiovascular solutions and consumer healthcare, Sanofi is committed to supporting the entire continuum of care for patients in over 170 countries worldwide. Its over 110,000 employees, distributed across approximately 100 countries, are working to produce innovative new therapeutics while simultaneously enhancing access to healthcare around the world. As a global leader, Sanofi has historically taken a proactive approach to tackling challenges to innovation and productivity head on, especially when it can help improve patient outcomes.

CHALLENGE
STREAMLINING AUTOXIDATION RISK ASSESMENTS IN DRUG FORMULATIONS

Developing the proper formulation of active ingredients (APIs) and excipients is almost as important in designing a new therapeutic as the APIs themselves. The wrong mix could result in the drug not being absorbed by the body, being absorbed at the wrong rate or being absorbed by the wrong tissue. Sanofi's challenge was removing the formulations bottleneck in its pharmaceutical development workflow by improving its autoxidation risk assessments of potential formulations. Autoxidation refers to the likelihood an API will react with ambient oxygen or trace impurities in the excipients, resulting in shorter shelf life, incorrect dosage, and reduced efficacy. If a potential API is susceptible to autoxidation, it has to undergo more testing to determine if this can be mitigated. Testing for autoxidation is often a laborious, manual process, as every potential formulation must be manually tested before it can pass to the next phase of development, clinical trials, and manufacturing scale up. Beyond creating a bottleneck for the pharmaceutical development team, the extensive physical testing required drives up unnecessary spend on materials and equipment. As a result, the pharmaceutical development team at Sanofi actively sought solutions to remove this bottleneck and create a leaner, more sustainable process.

THE SOLUTION
IN SILICO API SIMULATION IN BIOVIA MATERIALS STUDIO

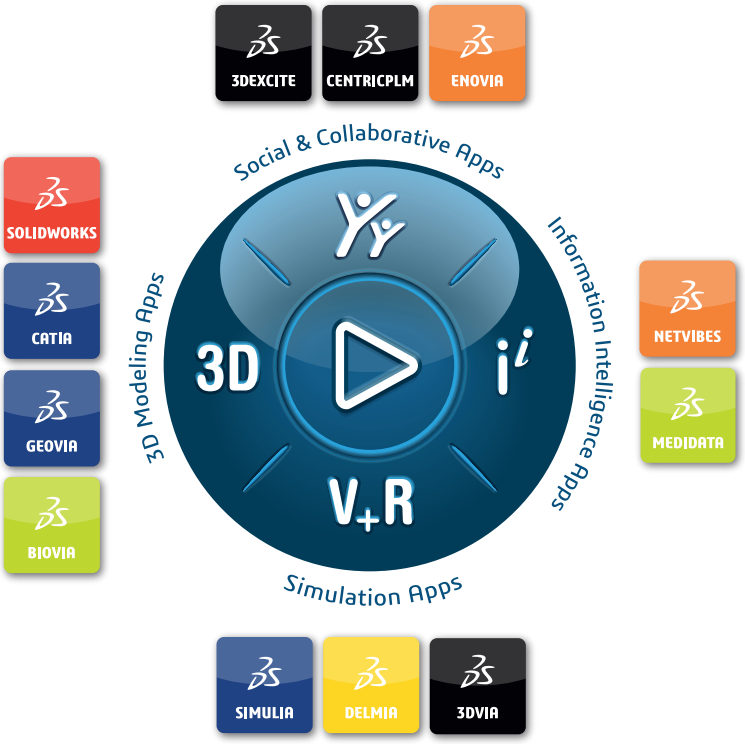
After exploring different materials modeling and simulation tools, Sanofi selected BIOVIA Materials Studio for its comprehensive collection of capabilities and overall user-friendliness. Through BIOVIA Pipeline Pilot, BIOVIA Materials Studio could be accessed as a web service through Sanofi's internal science portal, with both custom and ready-made protocols available to speed up predictive analyses and identify top candidates. This removed the need for "trial-and-error" driven experiments and maximized the value of scientists' time.

BIOVIA Materials Studio also assisted scientists with developing models to predict various materials properties such as bond disassociation energy with the DMoL^3 module and its collection of density functional theory (DFT) calculations. Scientists can select between various methodologies to optimize several parameters within the calculation such as speed or accuracy, depending upon their needs. Developing these models allows researchers to not only predict which substances are more likely to be a risk for autoxidation, it also helps them understand the nature of these degradation pathways to assist in the development of future formulations, further reducing the need for exhaustive physical tests

> "BIOVIA Materials Studio is now an integral part of our lead optimization workflow. It's saved us around six months of development time for each new API."
>
> — Dr. Philippe Lienard
> Business Development & CMC Discovery Coordinator, Sanofi

THE RESULT
A PROACTIVE AND EFFICIENT PHARMACEUTICAL DEVELOPMENT TEAM

Since implementing BIOVIA Materials Studio, Sanofi scientists on the pharmaceutical development team can determine the propensity of an API to autoxidize in its given formulation before running any physical experimentation. This has significantly shortened the cycle time needed to develop a new formulation by approximately six months. This proactive approach has also helped teams to better understand the properties of a formulation sooner, allowing them to focus on refining and optimizing the formulation rather than having to start over every time. This more streamlined approach to formulation design has lowered spend on physical resources by limiting the number of physical experiments needed to pass a formulation farther down the value chain. As a result, by leveraging BIOVIA Materials Studio Sanofi has optimized workflow efficiency, creating a more sustainable R&D organization and providing more positive outcomes to more patients faster.



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