

TASTY RESULTS: IMPROVING CHOCOLATE RECIPES WITH MATERIALS STUDIO

HOW FOOD & BEV R&D BENEFITS FROM
DATA-DRIVEN DECISION MAKING

USE CASE

THE CUSTOMER: A LEADING PRODUCER OF HIGH END CHOCOLATES

As a leading global player in the Food & Beverage industry, this BIOVIA customer values sustainability. Its employees recognize the impact that their organization has around the world, from farm to table. As a result, they seek to incorporate sustainable practices throughout the entire enterprise, responsibly sourcing raw materials and modernizing operations. Naturally, this philosophy also extends to their laboratories, where researchers actively explore new methods and technology to improve efficiency and shorten the time to discovery.

CHALLENGE: PREVENTING CHOCOLATE BLOOM

A key area for the customer's research is the prevention of chocolate bloom, a moldy looking white substance that occasionally forms on the surface of chocolate products. While decidedly not a health hazard, marketing research found that products that had bloomed would more frequently be perceived as being of poor quality and rejected by consumers. During the final step in the manufacturing process, called tempering, the temperature of the chocolate is precisely controlled to ensure uniform crystallization of the various ingredients. Bloom can arise from re-crystallization of cocoa butter on the surface of the product (fat bloom), or from the interaction of sugar ingredients with moisture (sugar bloom). This was a recurring problem in one of their leading chocolate products following a change in its manufacturing process. As a result, researchers needed to devise an altered recipe to minimize the likelihood of the chocolate blooming during storage.

The properties of chocolate are a delicate balance between the crystal size distribution, crystal shape, and crystal structure of its fat phase, which maintains the dispersion of solid particles such as sugar. It is theorized that bloom occurs when this crystal network converts to a different polymorph – a different arrangement of molecules within a crystal – due to temperature variations in manufacturing or storage. This can cause the fat phase to separate and cause the recrystallization seen in chocolate bloom. Often, emulsifiers and cocoa butter equivalents (CBEs), fats similar to the naturally occurring ones in chocolate,



**"BIOVIA Materials Studio
transformed the way we design
our products. Now we not only
understand how our products work,
we understand why they work."**

— Director of Product Development, Global Chocolate Producer

Challenge:

Product R&D relying too heavily on experimentation based on trial-and-error approaches caused delays in bringing new product formulations to market

Solution:

BIOVIA Materials Studio

Results:

- 20% reduction in laboratory experiments
- 10% faster formulation development
- Greater flexibility in reformulating products for different global markets
- Better understanding of macroscale product properties

are added to prevent this phase separation. However, optimizing this balance was a labor-intensive process for the customer's R&D team since their experimentation relied heavily on trial-and-error and the expertise of their senior staff. This led to increased product development times and higher costs, and the customer's management team realized that this empirical approach was no longer possible to remain competitive in the global market. As a result, they decided to adopt an *in silico* approach to screen out lower quality candidates prior to testing in the lab.

SOLUTION: PREDICTING POLYMORPH STABILITY WITH BIOVIA MATERIALS STUDIO

BIOVIA Materials Studio's native crystal polymorph prediction capabilities proved to be a perfect fit for this customer's needs. The Polymorph Predictor module utilizes a reliable Monte Carlo simulated annealing process to measure the energy of a variety of different crystal packing alternatives and to determine which, if any, are more thermodynamically stable than the original generated during the manufacturing process. If any of these more thermodynamically-stable polymorphs could easily lead to phase separation – and therefore chocolate bloom – scientists would need to reformulate their recipe. Previously, this would also require an extensive battery of characterization tests for each combination of cocoa butter, emulsifiers, and CBEs.

Using Materials Studio, scientists can now screen different combinations of cocoa butter triglycerides with various emulsifiers and CBEs *in silico* to predict which combinations would yield the ideal crystal lattice for preventing chocolate bloom prior to doing any tests in the lab, giving them more time to focus on the most promising candidates.

RESULTS: DATA-DRIVEN DECISIONS GUIDING FUTURE FORMULATIONS DESIGN

BIOVIA Materials Studio helps this customer more effectively explore the molecular interactions that yield the macroscale properties of their chocolate. With predictive modeling, their scientists can screen groups of candidates prior to testing in the lab, ensuring that only the formulations with the highest potential to succeed are tested. This approach has significantly impacted their work, providing a 20% reduction in laboratory experiments and accelerating their formulation development time by 10%. As a result, their team has more flexibility in optimizing their products' performance, and it leaves more time to develop formulations that are more targeted to the varying tastes of their different markets. This has allowed the customer to more effectively penetrate various global markets with a more consumer-centric approach.

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