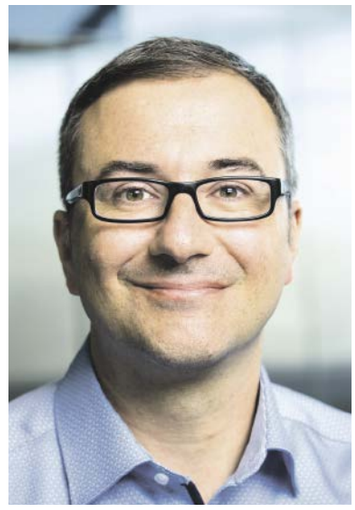
A Virtual Formulation Assistant

Leveraging Digitalization to Speed up Drug Product Development

The drug product development process can be time-intensive, costly, and has a high risk of failure. To help address the challenges of this laborious process, BASF has developed ZoomLab, a virtual formulation prediction and optimization tool. Currently, formulation is largely based on empirical methods with outcomes often depending on the expertise and intuition of individual formulators. With the aid of digitalization, formulators can have a significantly improved starting point and address certain challenges upfront rather than later, saving untold resources and mitigating risk of performance or stability failure. Ralf Kempf asked BASF's Ferdinand Brandl, Development Pharma Solutions, and Philipp Hebestreit, Technical Services Pharma Solutions Europe, about the technology and idea behind ZoomLab and how the virtual formulation assistant can speed up drug product development.



Ferdinand Brandl, Development Pharma Solutions, BASF

Philipp Hebestreit, Technical Services Pharma Solutions Europe, BASF

CHEManager: Where did the development of ZoomLab start? How did the idea for this virtual formulation assistant come up?

Ferdinand Brandl: The idea for ZoomLab comes from a workshop back in 2017. A few BASF colleagues met outside of their common office environment and brainstormed about different ways to make our customers' lives easier. Ultimately, we had the idea of developing a science-based formulation prediction system that provides our formulation experience in a progressive way and enables formulators to develop more robust drug formulations. In about a year and a half, we were able to bring this idea to life with ZoomLab.

When did you launch the first version of the platform?

F. Brandl: We launched the first version of ZoomLab in November 2019. The first version featured the Formulation Wizard, which is an easy-to-use tool that guides you through the process of identifying the best excipient combinations for a given drug substance. With the Formulation Wizard, our users create their own projects and receive a complete starting formulation based on the selected dosage form, the properties of the drug substance, and the desired target profile.

This version already included a tool that performs a risk analysis and recommends the best processing route for a given drug substance and another module that predicts the properties of a drug excipient combination.

How does ZoomLab work? How can it support formulators who use this tool?

Philipp Hebestreit: ZoomLab is built on a proprietary algorithm that simulates different ingredient combinations based on key parameters of a drug substance and the desired target dosage. The algorithm can predict the optimal formulation and provides step-by-step instructions on how to process it.

The main benefit for formulators is that the assistant, which we offer for free, is available 24/7. While other simulation tools take a significant amount of time to run predictions, ZoomLab provides immediate results. This helps reduce the number of time-consuming lab experiments by guiding the user to a scientifically optimized starting formulation.

Do users have to provide proprietary information about their product to get a useful result?

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P. Hebestreit: No. This is particularly important for our customers in the pharmaceutical industry. Formulators can fully utilize ZoomLab without providing proprietary information. The assistant does not require the formulator to disclose the name of the drug molecule or the chemical structure of the drug. Users just enter a few non-confidential physical properties of the drug substance and the target product dosages to let the tool provide predictions.

Additionally, the virtual assistant offers prepopulated drug substances from its database, but there is no obligation or need to enter the name of the drug substances at any time.

Does the assistant recommend exclusively BASF products?

F. Brandl: No, ZoomLab's algorithms are based on scientific publications; the formulation outcome is dictated by science. You will find a variety of substances in the assistant that are needed to create a starting formulation. The complete starting formulation is predicted using the most suitable excipients tailored to a drug formulation's specific needs, which includes chemistries beyond BASF's product portfolio.

Has the platform developed further since its launch?

F. Brandl: Yes, a lot. We have launched several updates of ZoomLab since version 1.0 was first released. To highlight a few features, we have introduced a content uniformity check, updated our excipient and formulation database, added an incompatibility check and integrated a tool which predicts the dissolution profile of the drug substance. Most recently, we launched ZoomLab 2.0 and added new modules that allow users to develop standard, protective, taste-masking, and enteric-release film coatings.

I recommend formulators sign up for our virtual formulation assistant and try out the different features. There's a lot more to explore.

How important is the feedback from users of this virtual assistant for the overall development of the platform?

P. Hebestreit: ZoomLab has been developed with the user experience in mind, and we continue to solicit and incorporate user feedback. This is particularly important because the assistant is continuously evolving. We normally launch an update every 1–2 months. User feedback helps us prioritize and develop the solutions we provide to our customers in each update.

What are your next plans for your tool? Which additional functions or components do you intend to add?

F. Brandl: ZoomLab is currently focused on oral solid dosage forms, but future releases are planned with additional dosage forms, manufacturing technologies, and more. For example, we will introduce additional features for topical dosage forms such as cream and ointments, and we are also working on features for sustained-release formulations.

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