

PRIMENA ZoomLab® VIRTUELNOG ASISTENTA U RAZVOJU DIREKTNO-KOMPRESIBILNIH FORMULACIJA: MOGUĆNOSTI I OGRANIČENJA

Ivana Vasiljević*, Ana Deljanin, Jovan Stojić, Erna Turković, Jelena Parojčić

Katedra za farmaceutske tehnologije i kozmetologiju, Univerzitet u Beogradu – Farmaceutski fakultet, Beograd, Srbija

*ivana.vasiljevic@pharmacy.bg.ac.rs

Razvoj lekova zahteva poznavanje složenih odnosa između karakteristika aktivnih supstanci (AS) i ekscipijenasa, procesnih parametara i ciljnog profila kvaliteta proizvoda, koje je teško pouzdano predvideti. Unapređenje naučnih saznanja u ovoj oblasti, dostupnost velikih baza podataka i primena mašinskog učenja doveli su do razvoja digitalnih platformi sa naprednim algoritmima koji podržavaju i omogućavaju brži razvoj formulacije.

U ovom istraživanju ispitivana je mogućnost primene platforme *BASF Virtual Assistant ZoomLab®* [1] kao alata za razvoj direktno-kompresibilnih formulacija, uz korišćenje kofeina i rivaroksabana kao model aktivnih supstanci. Sprovedena je uporedna analiza eksperimentalno dobijenih podataka i podataka integrisanih u platformu u okviru aplikacija *Tabletabilnost* i *Procesabilnost* aktivne supstance i tabletnih smeše, a potom faza razvoja formulacije, korišćenjem aplikacije *Formulation Wizard*.

Razmatranje svojstava AS u okviru platforme ukazivalo je na slabu procesabilnost, odnosno mogućnost obrade kofeina i rivaroksabana, što implicira na poteškoće prilikom direktne kompresije. Međutim, u aplikaciji *Formulation Wizard* predložen je sastav formulacija sa dobrom procesabilnošću. Formulacije, odabrane na osnovu predviđene povoljne protočnosti ili tabletabilnosti, pokazale su dobru gustinu, protočnost i kompresibilna svojstva, a izrađene tablete pokazale su zadovoljavajuće mehaničke karakteristike (čvrstina i friabilnost) i kratko vreme dezintegracije.

Zahvaljujući integrisanim algoritmima, kao i bazama podataka AS i ekscipijenasa, *ZoomLab®* platforma predstavlja koristan alat i vodič za razvoj formulacije. Međutim, baza ekscipijenasa ograničena je na odabrane proizvode kompanije BASF. Iako primena hibridnog pristupa može doprineti razvoju proizvoda u kraćem vremenu, uz manji utrošak materijala, potrebno je kritički razmotriti dostupne podatke i optimizovati sastav formulacije na osnovu sprovedenih eksperimenata.

Literatura

1. BASF Pharma. ZoomLab® – The Digital Platform for Drug Product Development <https://zoomlab.basf.com/>

Zahvalnica

Ovo istraživanje finansirano je od strane Ministarstva nauke, tehnološkog razvoja i inovacija Republike Srbije kroz dva Ugovora sa Univerzitetom u Beogradu – Farmaceutskim fakultetom broj 451-03-136/2025-03/ 200161 i broj 451-03-137/2025-03/ 200161.

EXPLORING THE BENEFITS AND LIMITATIONS OF THE ZoomLab® VIRTUAL ASSISTANT IN DIRECTLY COMPRESSIBLE FORMULATION DEVELOPMENT

Ivana Vasiljević*, Ana Deljanin, Jovan Stojšić, Erna Turković, Jelena Parojčić

Department of Pharmaceutical Technology and Cosmetology, University of Belgrade – Faculty of Pharmacy, Belgrade, Serbia

*ivana.vasiljevic@pharmacy.bg.ac.rs

Pharmaceutical development is based on complex relationships between active pharmaceutical ingredients (APIs) and excipients material properties, process parameters and targeted product performance which are difficult to model and predict. With advancement of the knowledge base in the field, availability of large datasets and machine learning, digital platforms have been created providing advanced algorithms to simplify and accelerate formulation development.

In this study, the applicability of BASF Virtual Assistant ZoomLab® [1], as a tool for development of directly compressible formulations was investigated, using caffeine and rivaroxaban as model drugs. Comparative evaluation of the experimentally obtained and built-in data has been performed using the API and Powder Blend *Tabletability* and *Processability* applications followed by *Formulation Wizard* guided formulation selection.

Based on API characteristics evaluation, both caffeine and rivaroxaban presented poor processability, indicating that direct compression into tablets would be challenging. However, *Formulation Wizard* identified a number of prospective formulations with good processability. Powder blends, selected based on predicted favorable flowability or tabletability, exhibited good flowability, powder density, and compression-related properties. The obtained tablets exhibited good mechanical properties (hardness and friability), as well as fast disintegration.

ZoomLab® built-in algorithms, as well as the API and excipient databases represent useful preformulation tool and provide insights which could guide formulation development. However, the excipients database is limited to the selected BASF products. Relevant outputs should be critically assessed and further optimized based on experimental observations leading to hybrid approach which would accelerate product development while minimizing time and resources consumption.

References

1. BASF Pharma. ZoomLab® – The Digital Platform for Drug Product Development <https://zoomlab.basf.com/>

Acknowledgements

This research was funded by the Ministry of Science, Technological Development and Innovation, Republic of Serbia through two Grant Agreements with University of Belgrade –Faculty of Pharmacy No 451-03-136/2025-03/ 200161 and No 451-03-137/2025-03/ 200161.