

Decision Support for Solubilization is now available in ZoomLab™

Poorly soluble drugs for oral administration present unique formulation challenges, particularly during early development. ZoomLab™'s “Decision Support for Solubilization” module helps formulators evaluate whether amorphous solid dispersions or lipid-based formulations are suitable dosage forms for your active ingredient!

ZoomLab™'s “Decision Support for Solubilization” module evaluates several parameters relevant for the structured development of poorly soluble drugs. Based on user-input experimental and computed properties, guidance on the following aspects is given:

- Estimated solubility in lipids
- Expected glass-forming ability
- Attainable drug load in solid dispersions
- Suitable formulation type based on classification algorithms
- Formulation examples of similar active ingredients

Based on the recommended formulation type, ZoomLab™ provides the user with further advice on subsequent formulation development.

Find the new “Decision Support for Solubilization” module on ZoomLab™'s homepage with the Solubilization modules.

Decision Support for Solubilization

Project Details

Project name (leave blank for default name): ZoomLab 2.4

Properties of Active Ingredient

Active ingredient (leave blank for new active ingredient): **Load data**

lipodien 50

Melting point (°C): 75.00

Glass transition temperature (°C): -45.00

Molecular properties of the active ingredient (enter values or import data from PubChem)

Molecular weight (g/mol)	206.28
Number of hydrogen bond acceptors	2
Number of hydrogen bond donors	1
Number of nitrogen atoms	0
Number of rotatable bonds	4
Number of non-aromatic double bonds	1
Number of aromatic six-membered rings	1
Computed partition coefficient (ALOGPS)	3.50
Topological polar surface area (A _{TPSA})	37.30
Hansen solubility parameters calculated by the van Krevelen method (MP ₁₂)	
Contribution from dispersion forces (δ _d)	17.85
Contribution from dipolar intermolecular force (δ _p)	2.22
Contribution from hydrogen bonds (δ _H)	7.15

Evaluation of Formulation Strategies

	Result
Estimated solubility in soybean oil	52.3 mg/g
Estimated glass-forming ability	poor
Proposed formulation (logistic regression model)	Lipid-based formulation
Share of solid dispersions (logistic regression model)	11.3%
Proposed formulation (decision tree model)	Lipid-based formulation
Share of solid dispersions (decision tree model)	0.0%

Based on molecular descriptors and comparison with available drug products, the logistic regression model proposes formulating the active ingredient as a lipid-based system. The decision tree model proposes formulating the active ingredient as a lipid-based system. Using molecular descriptors, the algorithm has identified the top 10 most similar active ingredients. Among these, 4 molecules are exclusively formulated as amorphous solid dispersions, and 2 molecules are exclusively formulated as lipid-based systems. Therefore, formulating the active ingredient as an amorphous solid dispersion or lipid-based system seems appropriate. In conclusion, based on the performed assessment, formulating the active ingredient as a lipid-based system is recommended.

Most Similar Drug Products

Achievable Drug Loading in Solid Dispersions

Graph showing LogP vs. Drug Loading (mg/g) for different formulation types. The active ingredient (marked with an 'X') is in the High drug loading (> 50%) region.

The glass transition temperature of the active ingredient is far from its melting point ($T_m - T_g = 14$). As a result, the maximum achievable drug loading in an amorphous solid dispersion is expected to be less than 50%. Please note that the classification is based on data from amorphous solid dispersions with HPMCAS. However, it is expected that the recommendations can be applied to solid dispersions in general.

Supplementary Information

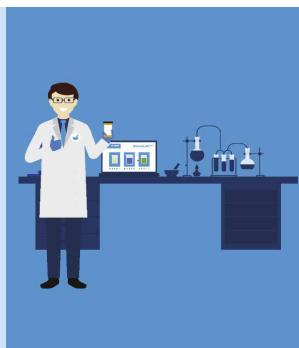
Formulation Advice

For lipid-based formulations, a systematic development approach is recommended due to the large number of excipients and potential combinations thereof. As a general rule, the target dosage strength should be compared to the expected solubility of the active ingredient in glycerols such as soybean oil. If the solubility is sufficient, solid-based systems with high oil content, such as oily solutions or SMEDDS, are viable options. If the solubility in glycerols is low, solvents based on polyethylene glycol or propylene glycol should be tested. If a suitable solvent or solvent mixture is identified, formulating the active ingredient as a SED (e.g., SED-based solid dispersions) or micellar systems (e.g., SED-type SED) can be considered. If no solvent or solvent mixture is identified, formulating the drug as an amorphous solid dispersion or nonaqueous system is an alternative.

Find excipients for lipid-based formulations

Discover for yourself how fast and easy it is to formulate with ZoomLab™ by signing up today – for free! Just enter a few physiochemical properties of the active ingredient and the target dosage form and let ZoomLab™ take care of the rest.

<https://info-mypharma.basf.com/>



**Register for a Webinar with
Pharma Excipients and BASF
ZoomLab™: Digitally guiding dosage form
and formulation for improved solubility**

Tuesday, June 8th, 2021
9AM EST | 3PM CET

Register at: <https://lnkd.in/d7ZhGJ6>