

Developability Classification of Active Ingredients is now in ZoomLab™

Formulation development normally begins with two questions:

- I) Can my active ingredient be formulated as an oral dosage form?
- II) And if so, can I rely on a conventional approach or is additional formulation work required to achieve sufficient oral bioavailability?

Developability Classification

Project Details
Project name (leave blank for default name)
ZoomLab 2.2

Definition of Target Profile
Dose of active ingredient (mg) * 400.00

Properties of Active Ingredient
Active ingredient (leave blank for new active ingredient)
Ibuprofen 50 (BASF) Load data

True density (g/mL) 1.12
d90 Value (µm) 126.50
Solubility in FaSSiF at 37 °C (mg/mL) * 2.10

Use effective intestinal permeability for calculation
 Predict effective permeability from molecular properties
Effective intestinal permeability (cm/s) * 2.13E-4

Computed properties of the active ingredient (enter values or import data from PubChem)
CAS registry no., chemical name, monograph name, or synonyms Search
Select compound Import

Molecular weight (g/mol) * 206.28
Computed partition coefficient (XLOGP3) * 3.50
Topological polar surface area (A²) * 37.30
Number of hydrogen bond donors * 1
Number of hydrogen bond acceptors * 2

Refresh results

Developability Classification
The active ingredient is assigned to DCS Class I

Parameter	Result
Predicted diffusion coefficient	8.88 × 10 ⁻⁶ cm ² /s
Dose number (Dn)	0.38
Absorption number (An)	2.2
Dissolution number (Dn)	15
Number of Lipinski's "Rule of Five" violations	0
Solubility limited absorbable dose (SLAD)	2272 mg
Max. d90 value for complete dissolution during intestinal transit	489 µm

Developability Classification System

Absorption number vs. Dose number graph showing DCS Class I region.

Formulation Advice
The topological polar surface area of the active ingredient is small (< 100 Å²). As a result, good intestinal absorption via paracellular diffusion is expected. No violations of Lipinski's "Rule of Five" were detected. Thus, based on the molecular structure, the oral bioavailability of the active ingredient is expected to be good. The particle size of the active ingredient should be below 489 µm to allow for complete dissolution during intestinal transit. The d90 value of the active ingredient is below this limit. Thus, complete dissolution of the active ingredient during intestinal transit is expected. The active ingredient is assigned to DCS class I. The active ingredient's particle size distribution, dissolution rate, solubility and permeability are not expected to be factors limiting oral bioavailability. Formulation of the active ingredient in a conventional or sustained-release dosage form (i.e., neat drug powder in capsule or tablet) is appropriate.

With the Developability Classification of Active Ingredients module, ZoomLab™ provides a handy tool that helps formulators answer these fundamental questions!

- Determine the Developability Classification System (DCS) class of active ingredients based on solubility, permeability and dose to be formulated.
- Estimate the permeability of an active ingredient from its molecular properties.
- Import data for selected ingredients from ZoomLab™'s database.
- Import computed properties conveniently from the PubChem® database.
- Estimate oral bioavailability based on the DCS class and computed molecular properties (e.g., Lipinski's Rule of Five, topological polar surface area).
- Obtain formulation advice according to the assigned classification (e.g., conventional vs. enabling formulation approach, recommendations on particle size and dose).

Find the new **Developability Classification of Active Ingredients** module on ZoomLab™'s homepage with the **Active Ingredients** modules.



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.

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