Lipophilicity

Balancing aqueous solubility, membrane passage, and drug exposure

NEZU
Biotech GmbH

Dear Client,

first and foremost, thanks for downloading this free resource. All graphics in this report are predictions made by our AI systems. They show the profile of this ADMET endpoint for thousands of marketed drugs. We divided it by indication, and as you can see, it changes a lot from one category to another. Therefore, try to find the closest indication to the compounds you are currently developing.

Lipophilicity shows how well a potential drug balances two needs: staying dissolved in body fluids and entering cells.

A drug must interact with both water and lipids. It must dissolve in blood and tissue fluids to move through the body. It must also cross biological membranes to enter cells and reach many drug targets. These membranes contain lipid bilayers. A compound that strongly prefers water may travel well in body fluids but cross membranes poorly. A compound that strongly prefers lipids may cross membranes well but dissolve poorly in aqueous fluids.

Scientists measure this balance using two liquids that do not mix:

- **n-Octanol**, which represents a lipid-like environment
- **Aqueous buffer**, which represents water-based body fluids

The compound is added to both liquids. The mixture is shaken and then allowed to separate into two layers. Scientists measure how much compound is present in each layer. The ratio is reported as logD at pH 7.4, a pH close to that of blood.

$LogD_{7.4}$ includes both the neutral and ionized forms of the compound. This makes it more informative than logP for molecules whose electrical charge changes with pH.

Very high lipophilicity causes poor aqueous solubility, strong plasma protein and tissue binding, nonspecific interactions, rapid metabolic clearance and greater toxicity risk.

Very low lipophilicity improves aqueous solubility but limits passive membrane permeability. This reduces oral absorption, tissue distribution and exposure to intracellular or brain targets.

Lipophilicity must be balanced. $LogD_{7.4}$ must be interpreted together with solubility, permeability, plasma protein binding and metabolic stability.

We generated these insights using advanced AI systems designed to analyze complex biotech data and highlight potential trends. While we strive for accuracy, AI models

can occasionally make mistakes or miss context, so please treat these predictions as informative guidelines rather than absolute facts.

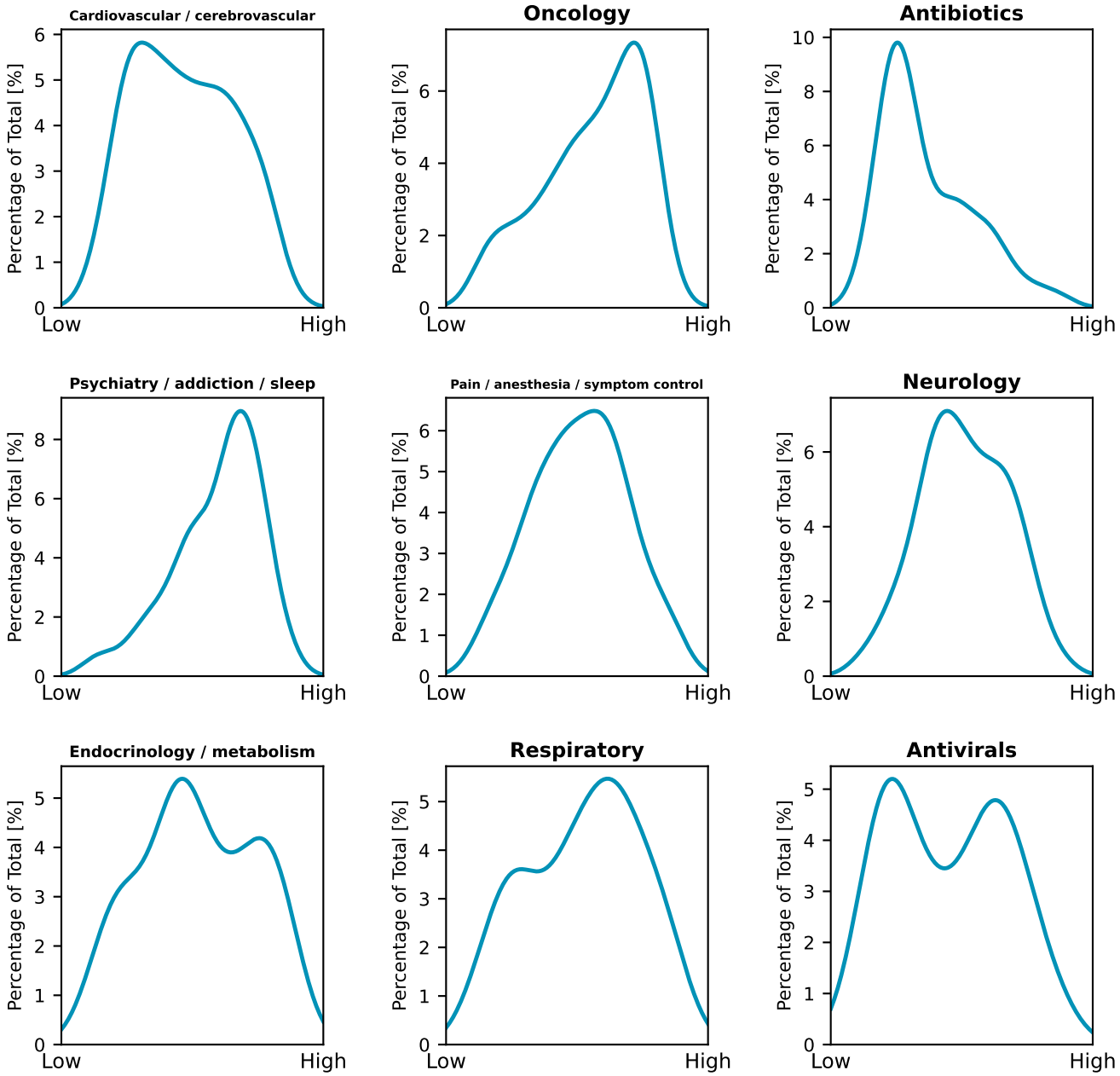
This report is provided for general informational and educational purposes only, not for medical diagnosis, treatment decisions, or financial advice. Because individual circumstances and data can vary, we cannot be held responsible for any decisions made or losses incurred based on these predictions.

Now that we got this out of the way, we genuinely hope these results are useful for your research.

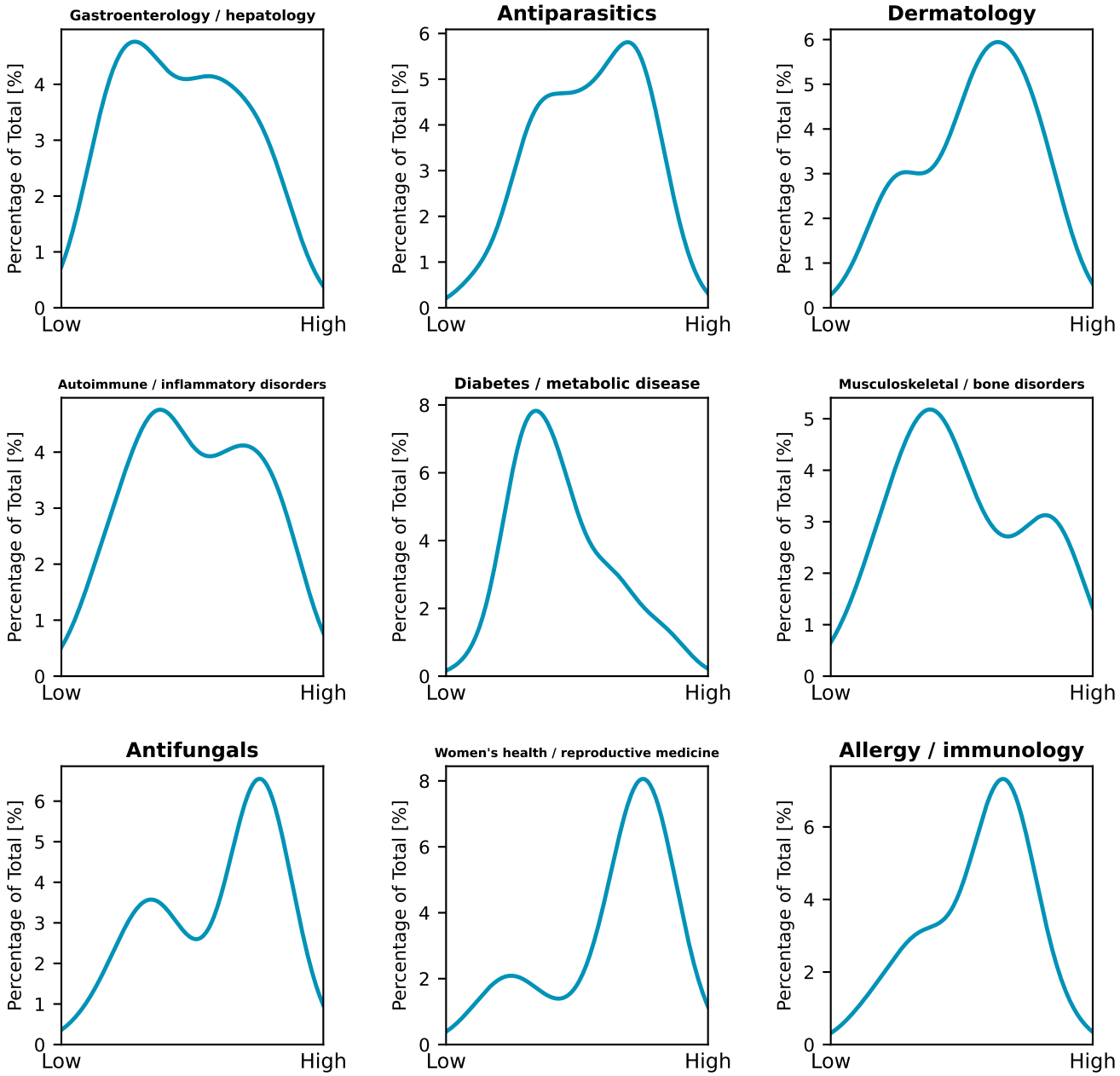
Sincerely,

Your friends at Nezu Biotech GmbH.

Lipophilicity



Lipophilicity



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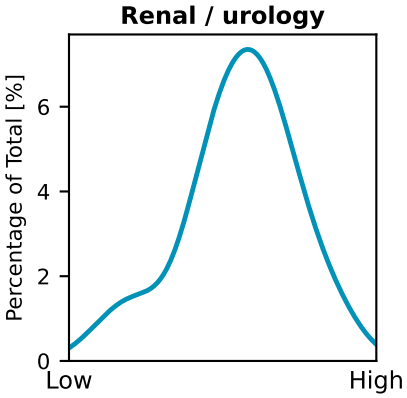

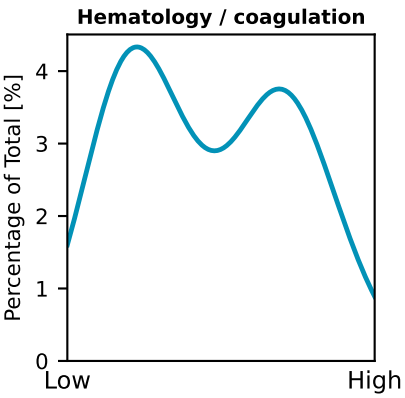

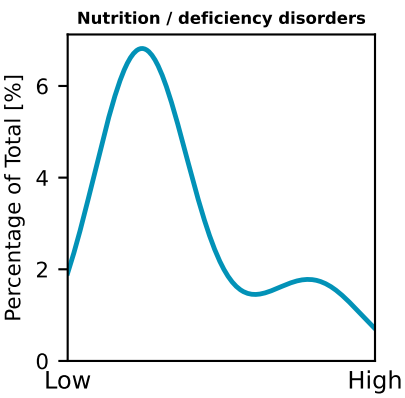

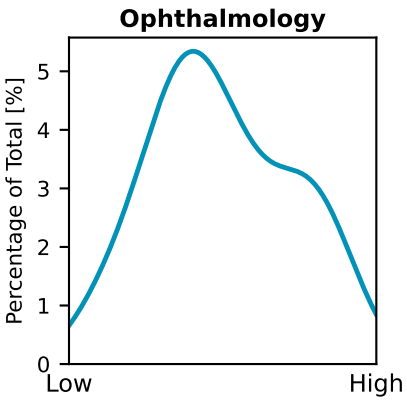

Derived from thousands of marketed drugs