Aqueous Solubility

Interpreting logS as a measure of compound dissolution in aqueous environments

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.

The **logS** answers how much of a compound dissolves in an aqueous liquid before the solution becomes saturated. A drug must dissolve before individual molecules can interact with biological targets, cross membranes, or become available for absorption. Poor aqueous solubility causes precipitation, unreliable assay results, difficult formulation, and limited exposure. However, greater solubility is not automatically better because highly soluble compounds can still have poor membrane permeability, rapid clearance, or weak target activity.

Solubility is commonly measured using an equilibrium or kinetic assay. In an equilibrium, or thermodynamic, experiment, excess solid compound is added to water or a defined buffer and mixed at a controlled temperature until the dissolved and undissolved material reach equilibrium. The remaining solid is removed by filtration or centrifugation. The dissolved concentration is then quantified, usually by high-performance liquid chromatography, ultraviolet spectroscopy, or mass spectrometry. Kinetic assays instead add a concentrated stock solution, often prepared in dimethyl sulfoxide, to an aqueous buffer and measure the concentration present before or after precipitation over a specified period.

Results are often reported as **logS**, the base-10 logarithm of molar solubility:

$\log S = \log_{10}(\text{solubility in mol/L})$.

Solubility reflects the balance between hydration of the dissolved molecule and the forces holding molecules together in the solid state. It depends on lipophilicity, molecular size, hydrogen bonding, crystal packing, salt form, temperature, pH, and ionization. For ionizable compounds, apparent solubility can change sharply with pH. Intrinsic solubility refers specifically to the neutral form.

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.

You have the vision. We can help make it reality.

Click here to book a demo. Tell us about your molecules.

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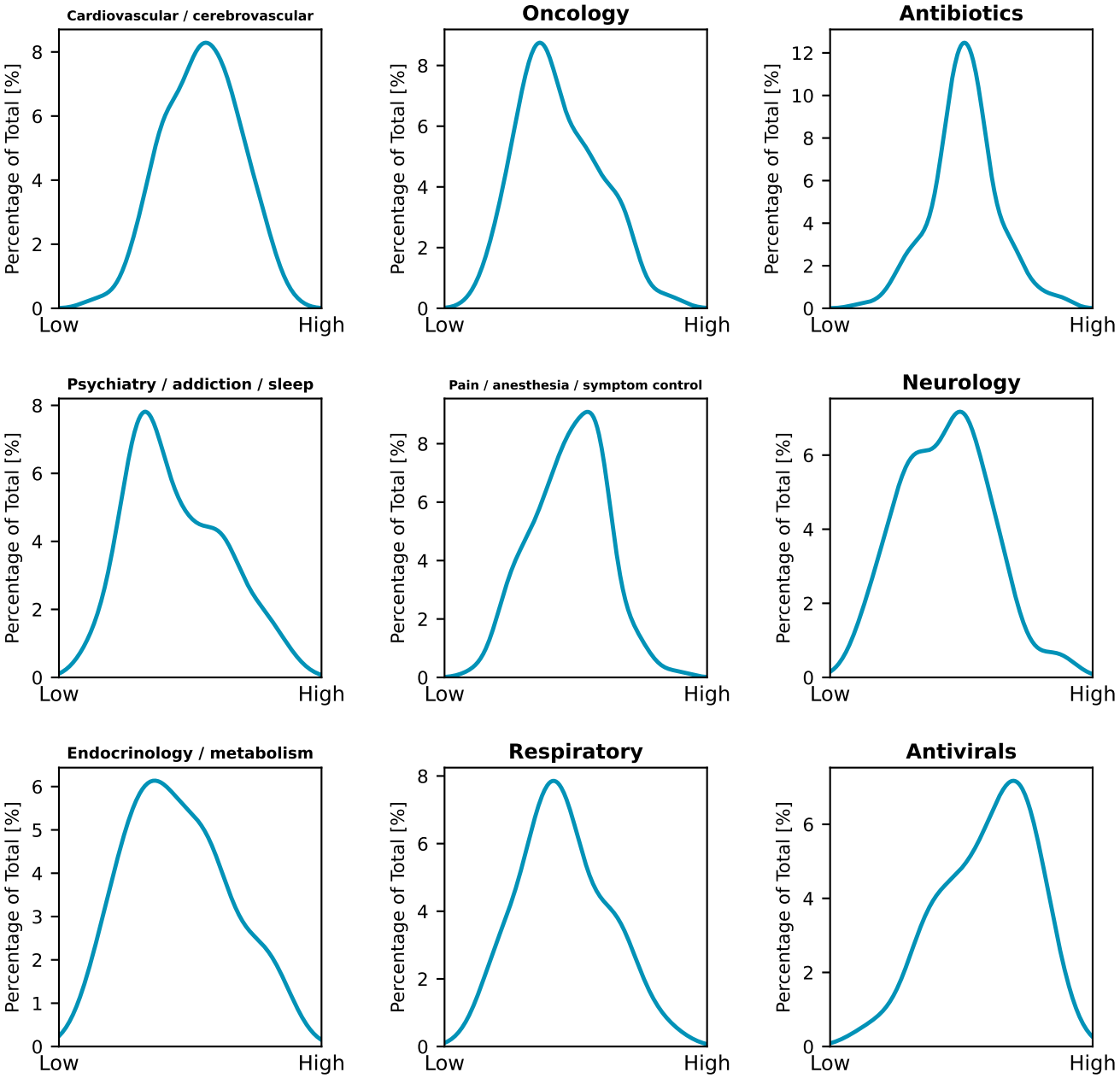
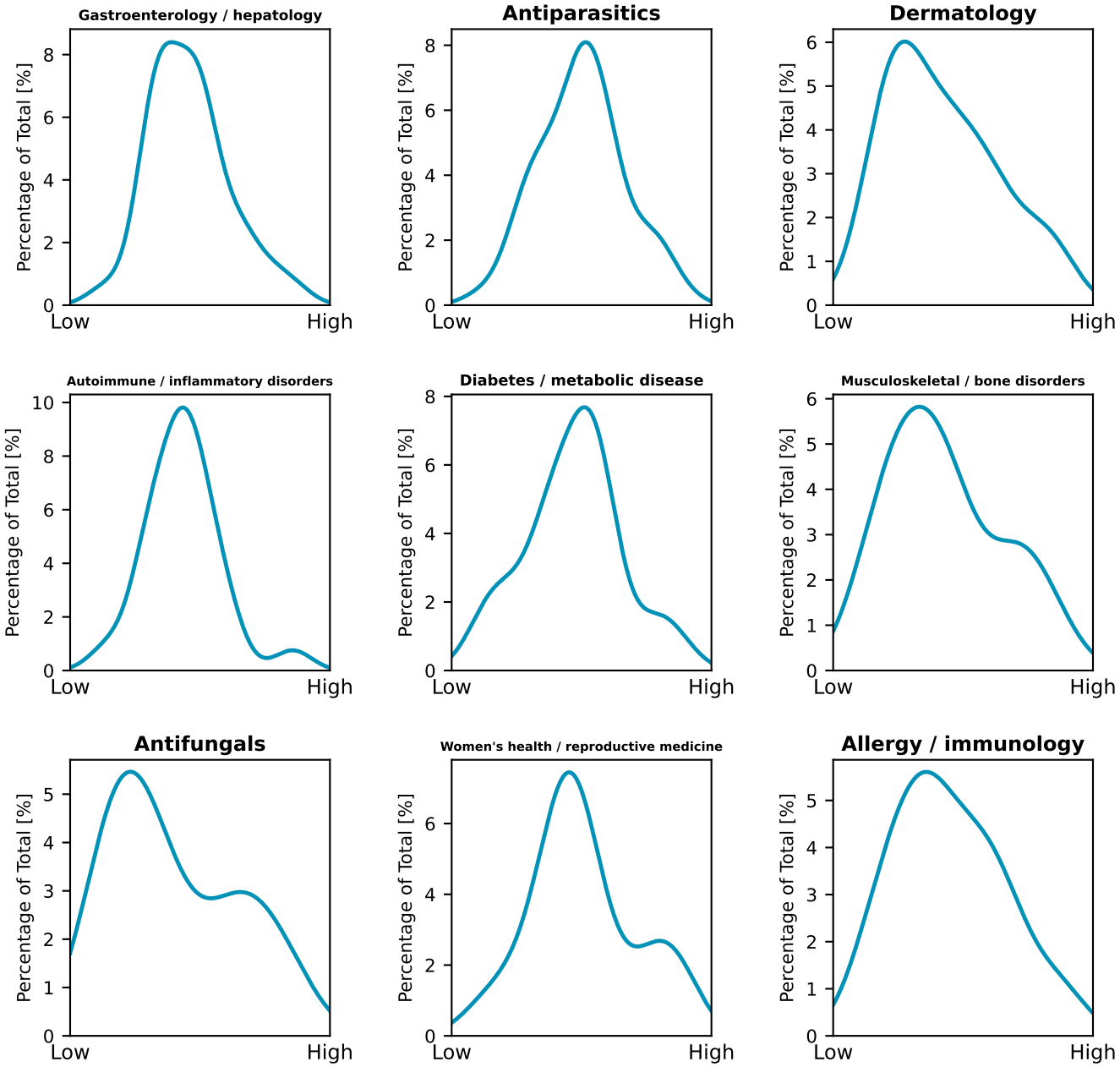
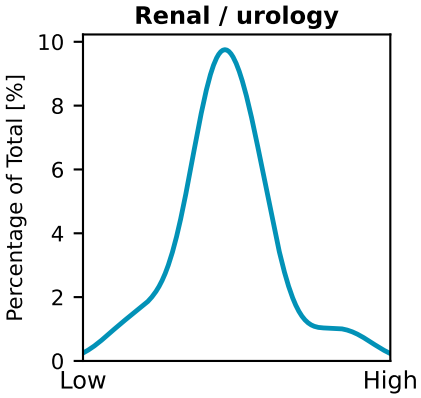
logS

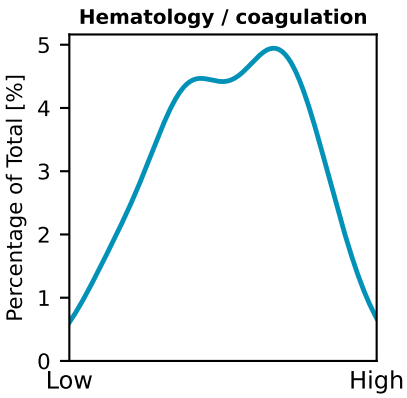


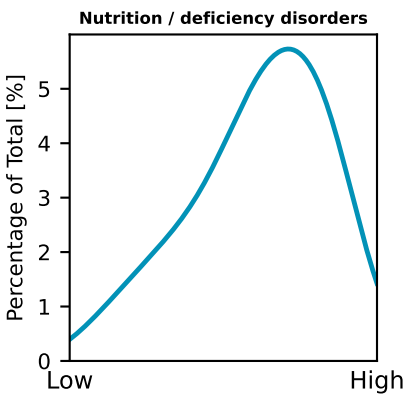
logS

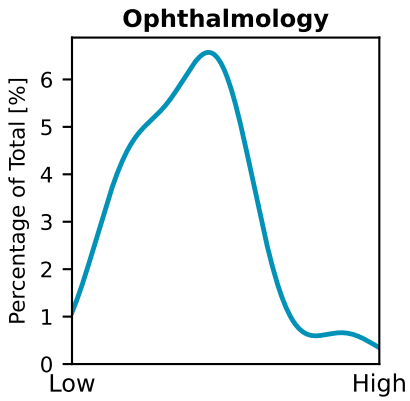

Gastroenterology / hepatology
Antiparasitics
Dermatology
Autoimmune / inflammatory disorders
Diabetes / metabolic disease
Musculoskeletal / bone disorders
Antifungals
Women's health / reproductive medicine
Allergy / immunology
Percentage of Total [%]
Low
High
Derived from thousands of marketed drugs

logS









Derived from thousands of marketed drugs