

AP ADMET Predictor®

Predict and build with confidence

Beyond Rule of Five (bRo5)

Natural language inquiries

Summarize the predicted ionization state for cetrizine at pH 3.0 and create the % ionized vs. pH plot

Embedded ADMET Modeler functionality

HTPK Simulation Results — IV Bolus
Compound: N#C(=O)NC(Cc1cc(C)ccc1)ccc(C)C(=O)N
Species: Human | Dose: 10 mg | Route: IV Bolus

Bioavailability

Property	Value	Notes
%Fa	100.00%	Expected for IV — bypasses GI absorption
%Fb	100.00%	Expected for IV — no first-pass metabolism

Exposure & Pharmacokinetics

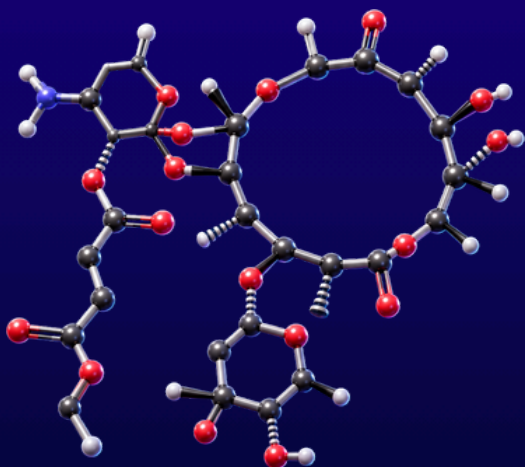
Property	Value	Units	Description
Cmax	26.41	ng/mL	Peak plasma concentration (at t = 0 for IV bolus)
Cmin	5.84	ng/mL	Trough plasma concentration
AUC	324.51	ng·h/mL	AUC for the dosing interval

Predict the oral bioavailability in humans for a 10 mg tablet dose of the compound with the SMILES: O=C(Oc1c(C(=O)O)ccc1)C

Display the major CYP metabolites of alprazolam and highlight the hotspots

From the leaders in ADMET prediction...

Trusted by computational chemists, medicinal chemists, and DMPK scientists worldwide, ADMET Predictor helps teams evaluate molecular properties earlier, design stronger candidates, and make informed decisions throughout discovery.



What's NEW in version 14?

- Work with Intelligent Scientific Guidance**
Accelerate modeling and workflows with AI-assisted guidance to execute operational tasks, generate and analyze results, and gain insights from vast amounts of domain-specific content.
- Build Smarter Models**
Automate the creation and retraining of models as data is generated, and leverage novel and/or custom descriptors to help your science evolve as new discoveries emerge
- Explore More Challenging Chemistry**
Extend trusted predictions to Beyond Rule of 5 compounds with expanded prediction coverage for increasingly complex molecules
- + More!**

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