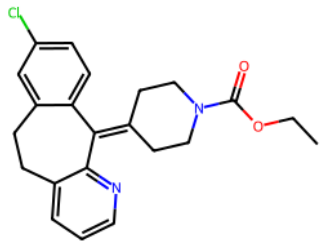
# Astinova AI Platform — ADMET Profiling Report

Subject: Loratadine (public reference compound) · in silico ADMET across absorption, distribution, metabolism, excretion, toxicity

Model-based predictions, expert-reviewed. Illustrative sample on a public molecule.




| | |
|---|---|
| **MW (Da)** | 382.9 |
| **logP** | 4.89 |
| **TPSA (A²)** | 42.4 |
| **HBD / HBA** | 0 / 3 |
| **QED** | 0.70 |
| **Lipinski violations** | 4 |

SMILES: CCOC(=O)N1CCC(=C2c3ccc(Cl)cc3CCc3cccnc32)CC1

## Absorption

| Endpoint | Value | Interpretation |
|---|---|---|
| Human intestinal absorption (prob) | **1.000** | High |
| Caco-2 permeability (log cm/s) | **-4.59** | Permeable |
| Oral bioavailability (prob) | **0.685** | Favourable |
| Aqueous solubility (log mol/L) | **-4.85** | Low solubility |

## Distribution

| Endpoint | Value | Interpretation |
|---|---|---|
| BBB permeability (prob) | **0.955** | Predicted BBB-permeable |
| P-gp substrate (prob) | **0.700** | Low efflux |
| Plasma protein binding (%) | **96.9** | Highly bound |

## Metabolism (CYP)

| Endpoint | Value | Interpretation |
|---|---|---|
| CYP3A4 inhibitor (prob) | **0.663** | Lower risk |
| CYP2C9 inhibitor (prob) | **0.861** | DDI risk |
| CYP2D6 inhibitor (prob) | **0.355** | Lower risk |

## Excretion & toxicity

| Endpoint | Value | Interpretation |
|---|---|---|
| Half-life (Obach, h) | **47.6** | Model estimate |
| hERG inhibition (prob) | **0.684** | Moderate |
| DILI (prob) | **0.747** | Hepatotoxicity flag |
| AMES mutagenicity (prob) | **0.080** | Low |
| Clinical toxicity (prob) | **0.089** | Low |
| Carcinogenicity (prob) | **0.089** | Low |
| LD50 (log mol/kg) | **2.90** | Moderate acute tox. |

Predictions are in silico estimates generated by the Astinova AI Platform and reviewed by a chemist. Probabilities are model outputs, not experimental values; hERG, DILI, and CYP flags should be confirmed with the corresponding in vitro assays before decision-making.