

Literature evidence

Task-level preparation

Target property
Oral bioavailability

Deep research
Identify relevant factors

Factors / evidence groups

Absorption

Intestinal transport

Liver clearance

...

Guide indirect searches

Starling

Search · extract · standardize

Evidence Corpus



Direct outcome



Indirect Absorption



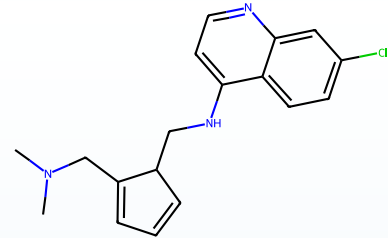
Indirect Transport



Indirect Metabolism

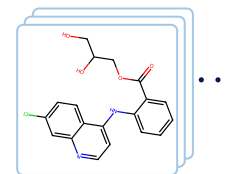
Context optimization

Query q · structure only



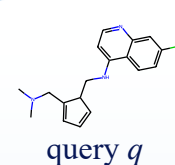
4-aminoquinoline derivative
No observed property

Retrieved record (from corpus)



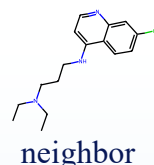
Learned transfer model

Same property, different molecules



query q

Transfer score



neighbor

Select evidence context

Transfer score



Informativeness



Molecular similarity



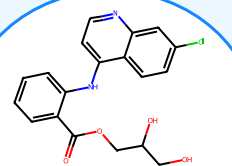
Diversity

Selected evidence context

Analogical reasoning

Example: oral bioavailability

Direct outcome



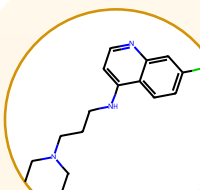
Glafenine

Direct

Human oral $F \approx 33\%$

Shared core:
supportive analogy

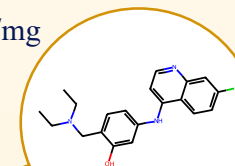
Liver clearance



AQ-13

Low liver-microsome clearance
Human $CL_{int} < 7 \mu L/min/mg$

Supports limited first-pass loss

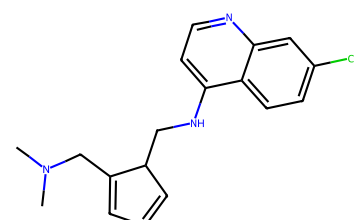


Isoquine

High first-pass metabolism
N-diethylamino side chain

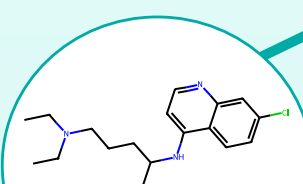
Downweighted:
metabolic site absent in q

Query q



4-aminoquinoline derivative
No observed property

Absorption

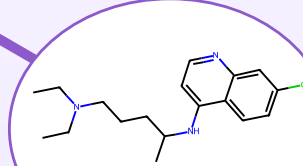


Chloroquine

High Caco-2 permeability
 $20 \times 10^{-6} \text{ cm/s}$
pH 7.2

Supports absorption

Intestinal transport



Chloroquine

No P-gp substrate signal
In the reported Caco-2 assay

Supports limited efflux

Prediction: high oral bioavailability

$F \geq 20\%$ · moderate confidence

Shared-core evidence outweighs a side-chain-specific liability.

Color: evidence group

● Direct ● Absorption / permeability

● Intestinal transport ● Liver clearance

— Solid: supportive analogy

- - - Dashed: downweighted

LLM assessment:
compare structural and mechanistic evidence from related molecules.