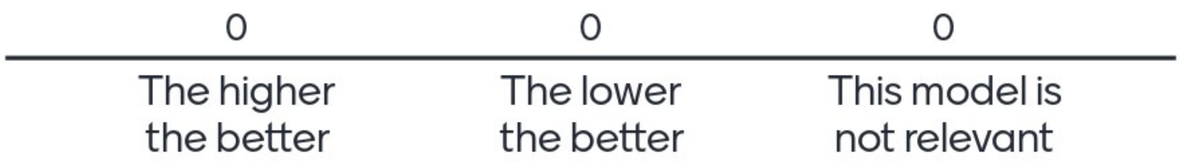
Recap from yesterday's session

Antimalarial compounds in ChEMBL and COCONUT

Mentimeter

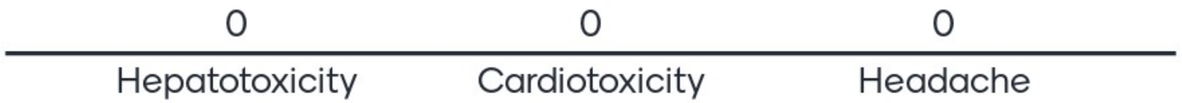
The output of the MMV antimalarial model eos2rta...



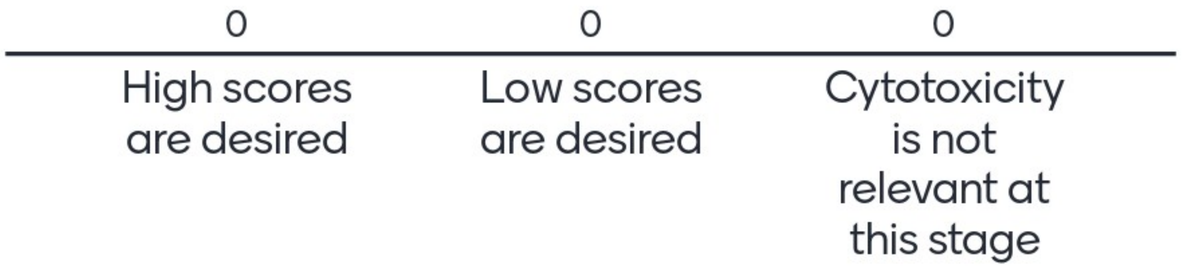
The antimalarial model eos7yti, built with Open Source Malaria series 4 data, is likely to

0	0	0
Be applicable to a broad chemical space	Be accurate only with molecules series 4 molecules	Be most useful in a lead optimization stage

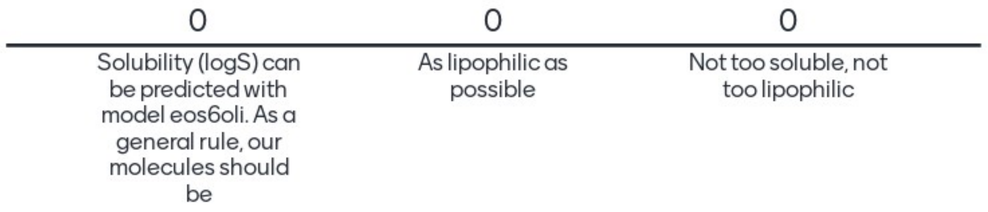
Interaction with the hERG ion channel, as predicted with model eos4tcc, can cause



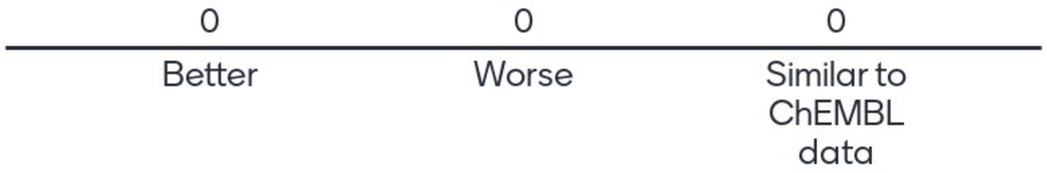
The model eos3le9 predicts liver cytotoxicity and it is a classification, therefore



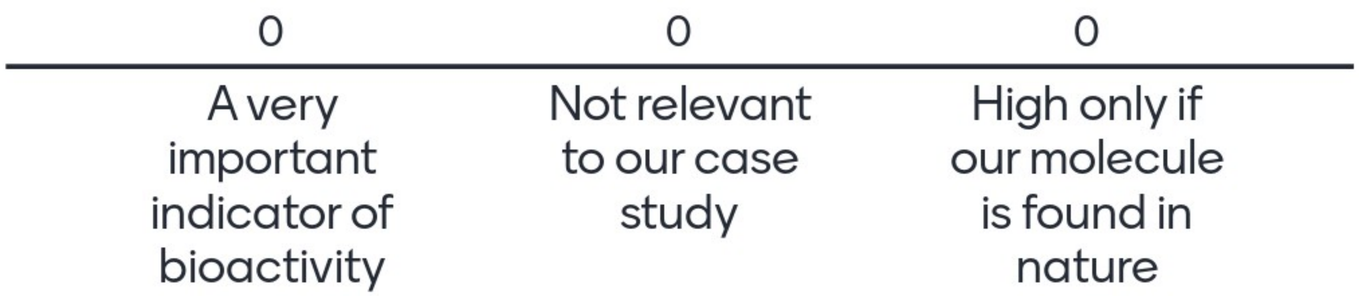
Solubility (logS) can be predicted with model eos6oli. As a general rule, our molecules should be



Synthetic accessibility (SA) of a compound can be quantified with model eos9ei3. In COCONUT, we expect SA to be



The NP-likeness score (eos9yui) is



Rank the models by importance (ranking quiz question)

1st	eos4rta (MMV)
2nd	eos7yti (OSM)
3rd	eos6oli (solubility)
4th	eos4tcc (cardiotoxicity)
5th	eos3le9 (cytotoxicity)
6th	eos9ei3 (synthetic accessibility)
7th	eos9yui (natural product)