

#### Recap from yesterday's session

Antimalarial compounds in ChEMBL and COCONUT



#### The output of the MMV antimalarial model eos2rta...

0	0	Ο	
The higher	The lower	This model is	
the better	the better	not relevant	

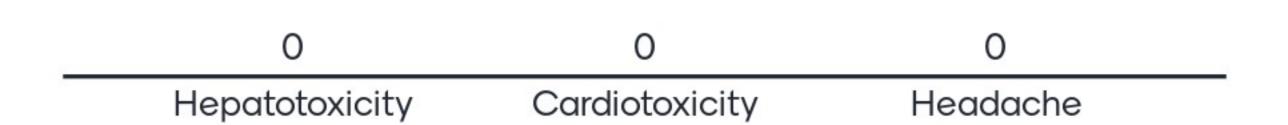


## The antimalarial model eos7yti, built with Open Source Malaria series 4 data, is likely to

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

0	Ο	Ο
High scores are desired	Low scores are desired	Cytotoxicity is not
		relevant at this stage



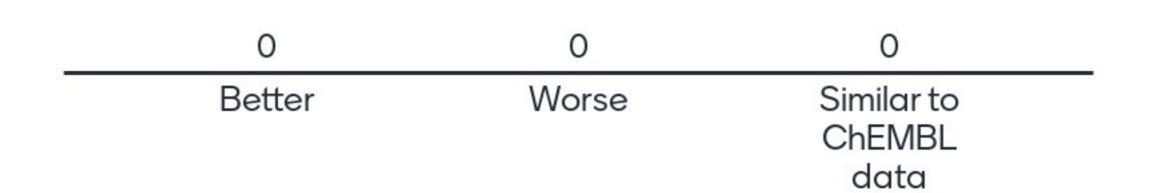
# Solubility (logS) can be predicted with model eos6oli. As a general rule, our molecules should be

O O O

Solubility (logS) can As lipophilic as be predicted with possible too lipophilic 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

	)	0		0
Av	ery	Not releva	nt H	igh only if
impo	rtant	to our cas	e ou	r molecule
indica	ator of	study	is	found in
bioad	ctivity			nature

### Rank the models by importance (ranking quiz question)

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1steos4rta (MMV)2ndeos7yti (OSM)3rdeos6oli (solubility)4theos4tcc (cardiotoxicity)5theos3le9 (cytotoxicity)6theos9ei3 (synthetic accessibility)7theos9yui (natural product)
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