

# In Silico ADMET prediction - ZeptoWard

*Commonly used acronym: ZeptoWard*

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## Organisation

**Name of the organisation** Kantify

**Department** Drug Discovery Department

**Country** Belgium

## SCOPE OF THE METHOD

<b>The Method relates to</b>	Human health
<b>The Method is situated in</b>	Translational - Applied Research
<b>Type of method</b>	In silico

## DESCRIPTION

### Method keywords

ADMET

absorption

distribution

Metabolism

excretion and toxicology

### Scientific area keywords

machine learning

artificial intelligence

bioinformatics  
computational biology

## **Method description**

ZeptoWard is a Machine Learning solution (AI) which identifies the ADMET properties of compounds. It can accurately predict over 80 properties related to absorption, distribution, metabolism, excretion, and toxicity properties, how a specific compound or combination of compounds will perform. It can also identify off-target effects of compounds. Because it runs *in silico*, it can feasibly be run on a full library, rather than only on lead compounds, making it a unique solution to optimize leads and decreasing the risks of drug discovery efforts.

## **Method status**

Published in peer reviewed journal

## **PROS, CONS & FUTURE POTENTIAL**

### **Advantages**

ZeptoWard is novel and unique in the following ways :

- It can predict ADMET properties across 80 endpoints and enable drug researchers to proactively mitigate unknown effects during the lead optimization phase;
- As it is pre-trained on large datasets, it does not need anterior data to generate results.
- For the above reason, ZeptoWard can generate results in a matter of minutes, for any compound.
- It can help drug discovery teams optimize the ADMET properties of their compounds.
- Last, but not least, it has a very high performance and is therefore a reliable solution to accelerate the work of drug researchers.

Benefits: By using ZeptoWard we can:

- Decrease risk of drug discovery and development by identifying unwanted properties early on;
- Increase chances of success during clinical validation;
- Minimize animal testing to compounds that have a promising ADMET profile;
- Decrease costs of lead optimization through a powerful, fast ADMET property

analysis;

- Speed up time to market by optimizing the ADMET properties early on. For proper lead optimization, ZeptoWard can be complemented by its sister solution ZeptoHit, which identifies ADMET properties of lead compounds.

## Challenges

ZeptoWard is probabilistic, even if its accuracy and speed is considerably higher than the state of the art. This means that its predictions obviously need to be validated, starting with mechanistic or phenotypic assays.

## Modifications

ZeptoWard is constantly improved.

## REFERENCES, ASSOCIATED DOCUMENTS AND OTHER INFORMATION

### References

<https://www.frontiersin.org/articles/10.3389/fphar.2022.856804/full>

### Links

[Learn more about ZeptoWard](#)

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