In Silico ADMET prediction - ZeptoWard

Commonly used acronym: *ZeptoWard*
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SCOPE OF THE METHOD

The Method relates to	Human health
The Method is situated in	Translational - Applied Research
Type of method	In silico
This method makes use of	Animal derived cells / tissues / organs

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.

Lab equipment

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

Associated documents

Links

Learn more about ZeptoWard

PARTNERS AND COLLABORATIONS

Organisation

Name of the organisation Kantify

Department Drug Discovery Department

Country Belgium

Geographical Area Brussels Region

Coordinated by

Financed by