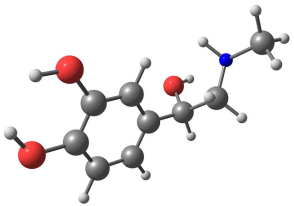
UNIVERSITY OF CAMBRIDGE

Applied machine learning to accelerate development of formulations and chemical processes

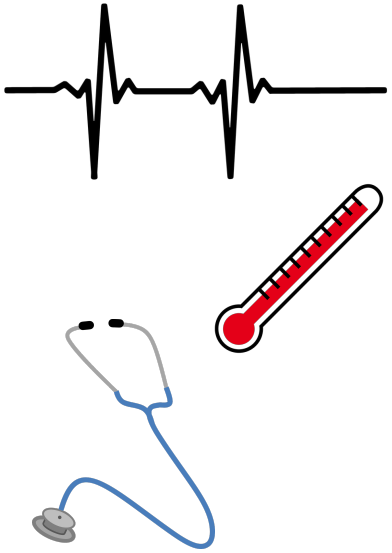
Gareth Conduit

Black box machine learning for drug design

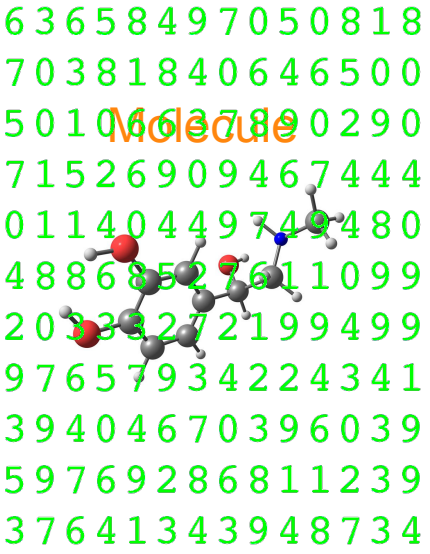
Molecule

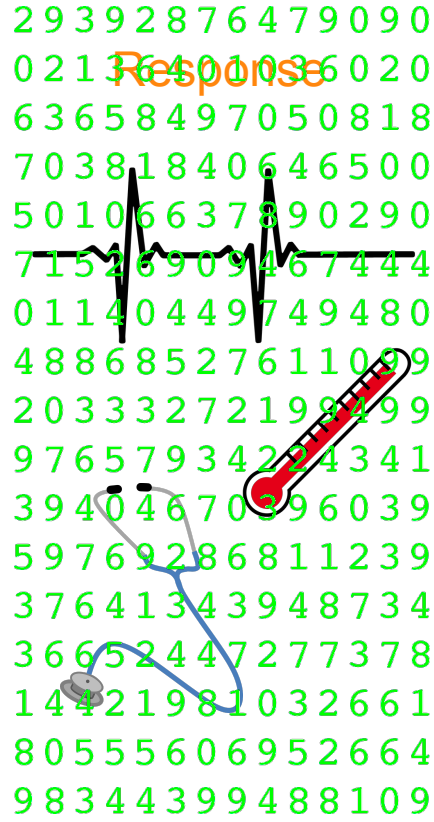


Response



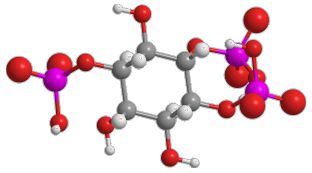
Train the machine learning





Predict behavior of new drug

Molecule



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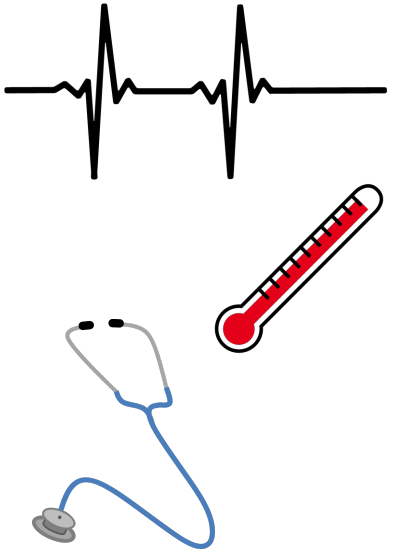
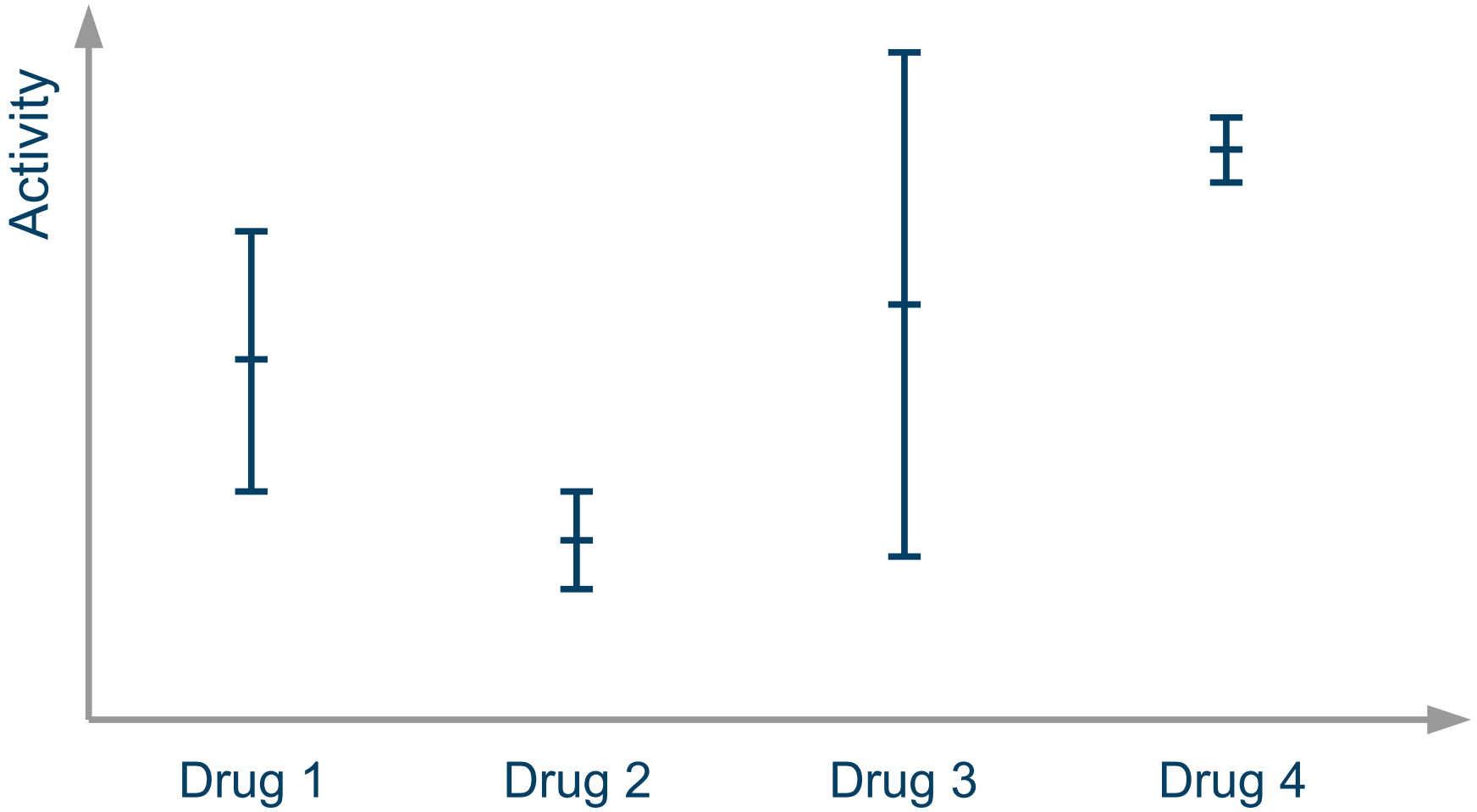


Open Source Malaria contest

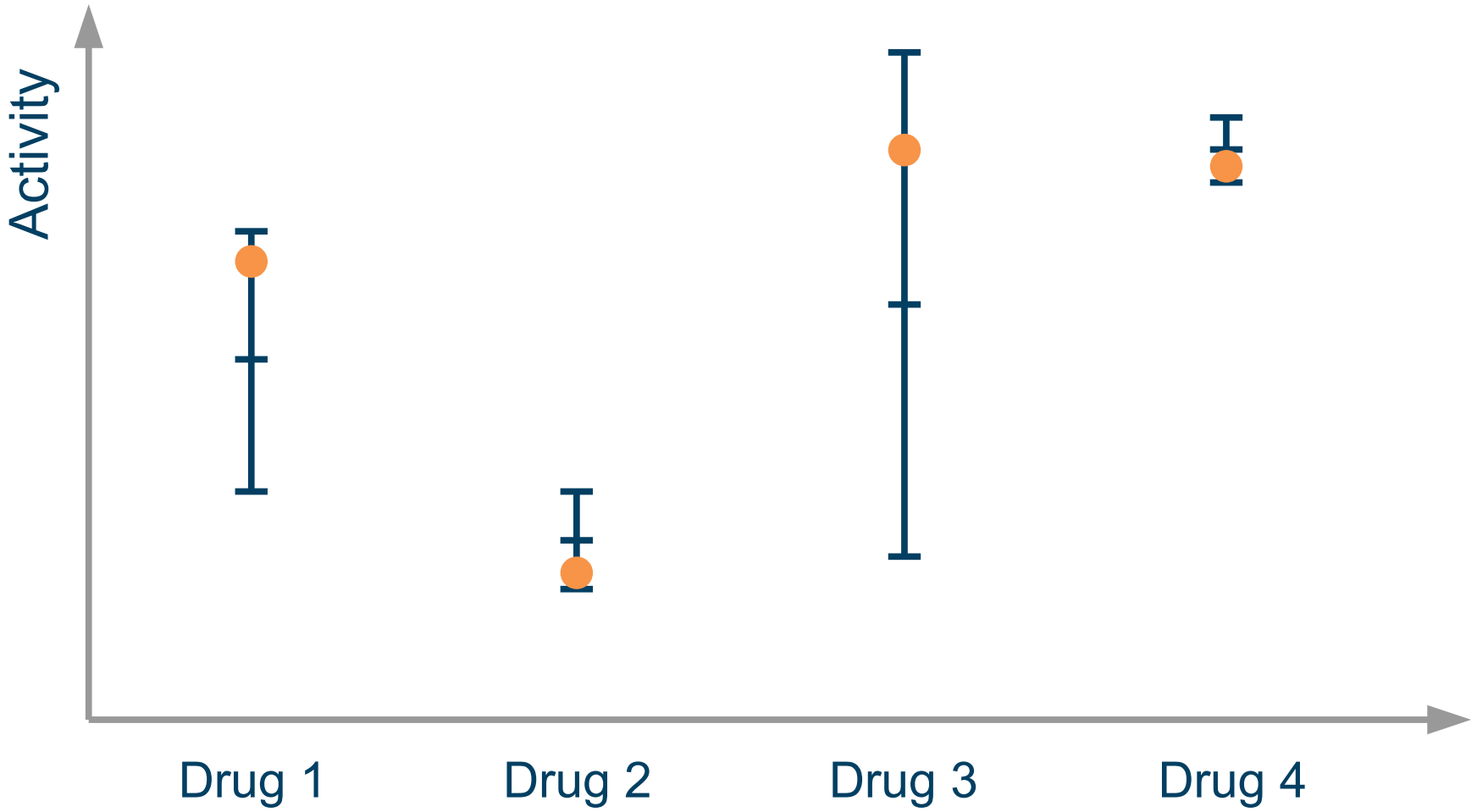
OPEN SOURCE MALARIA

Looking for New Medicines

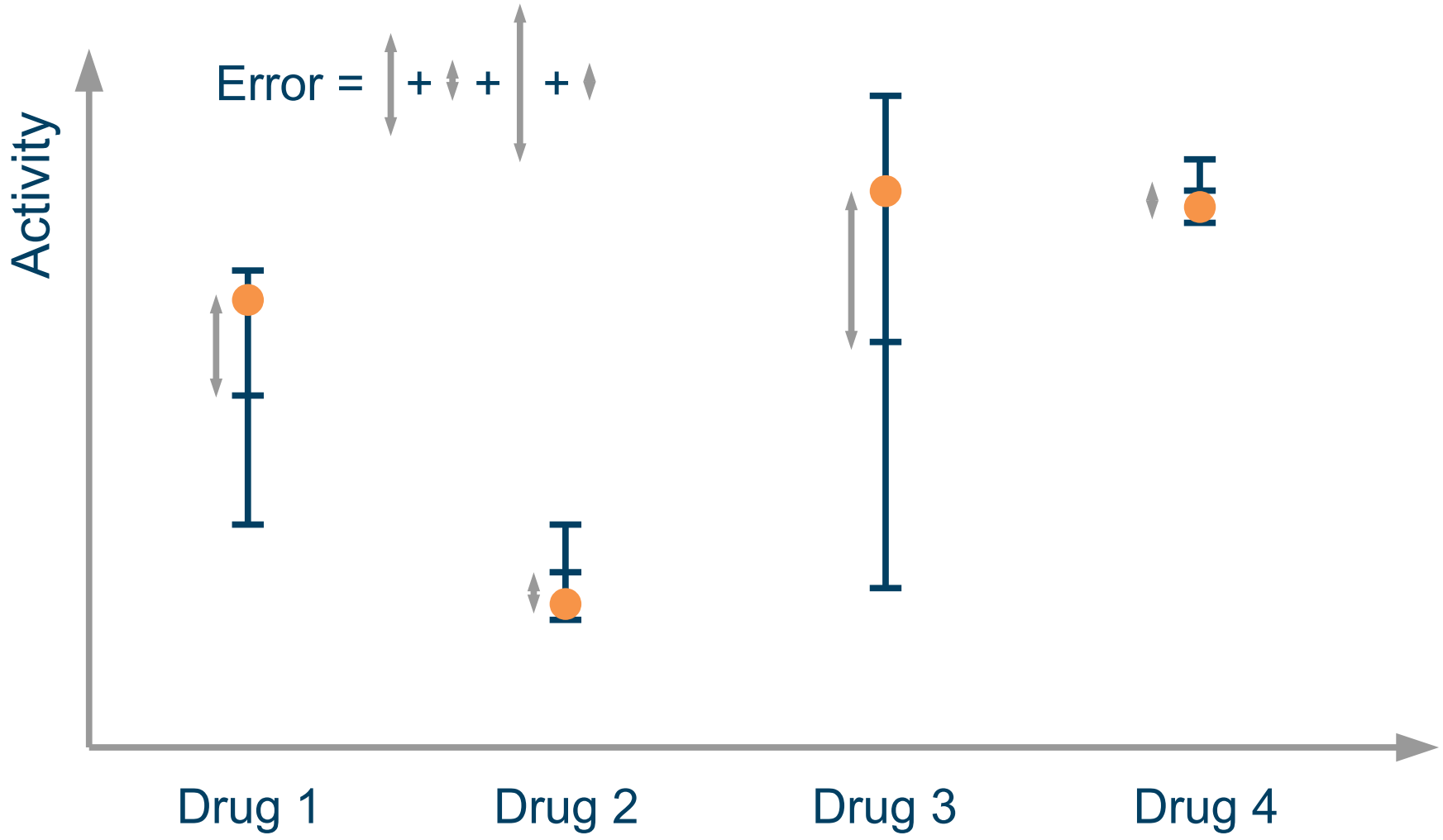
Predictions have an uncertainty



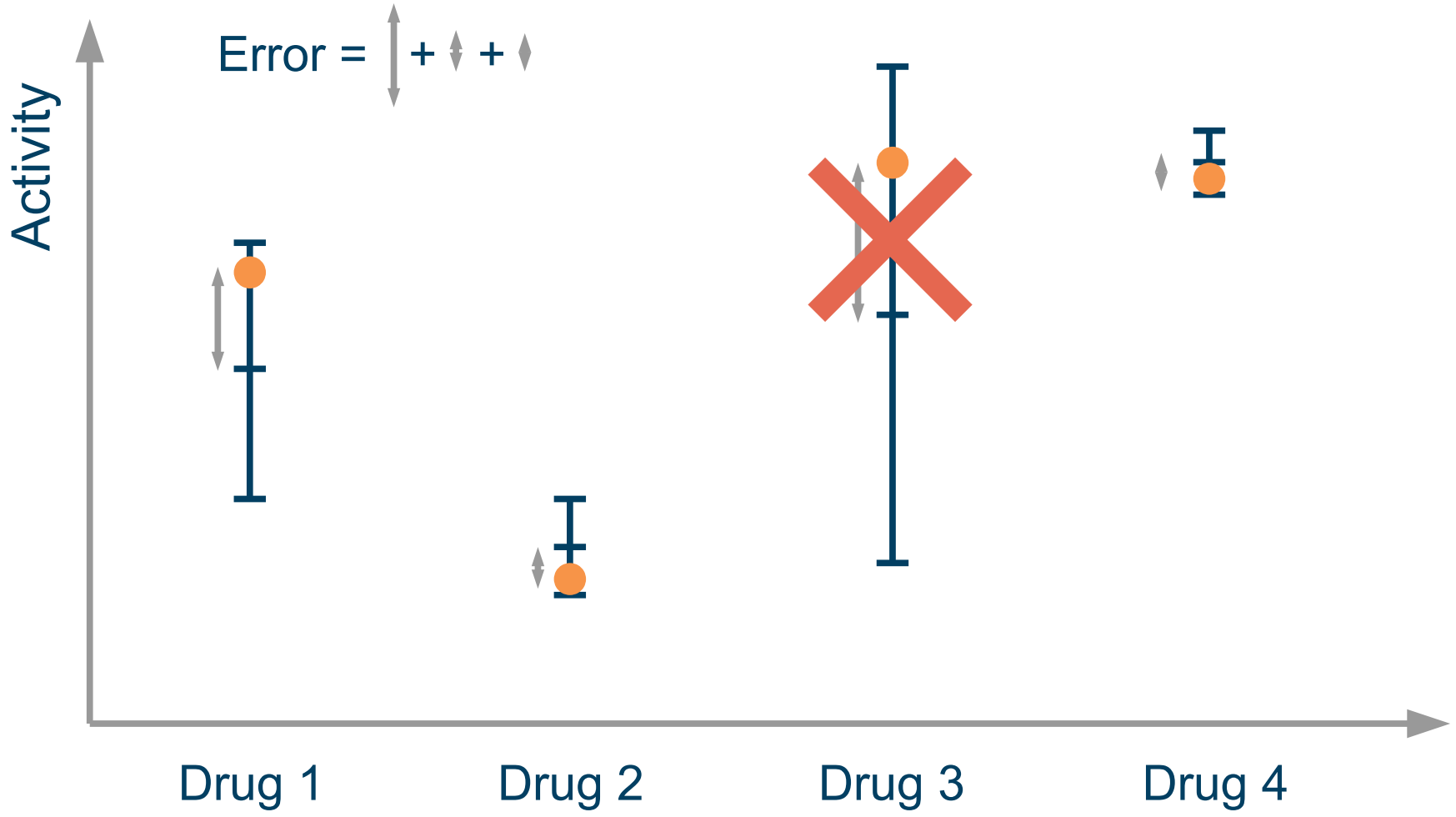
Validation data typically within one standard deviation



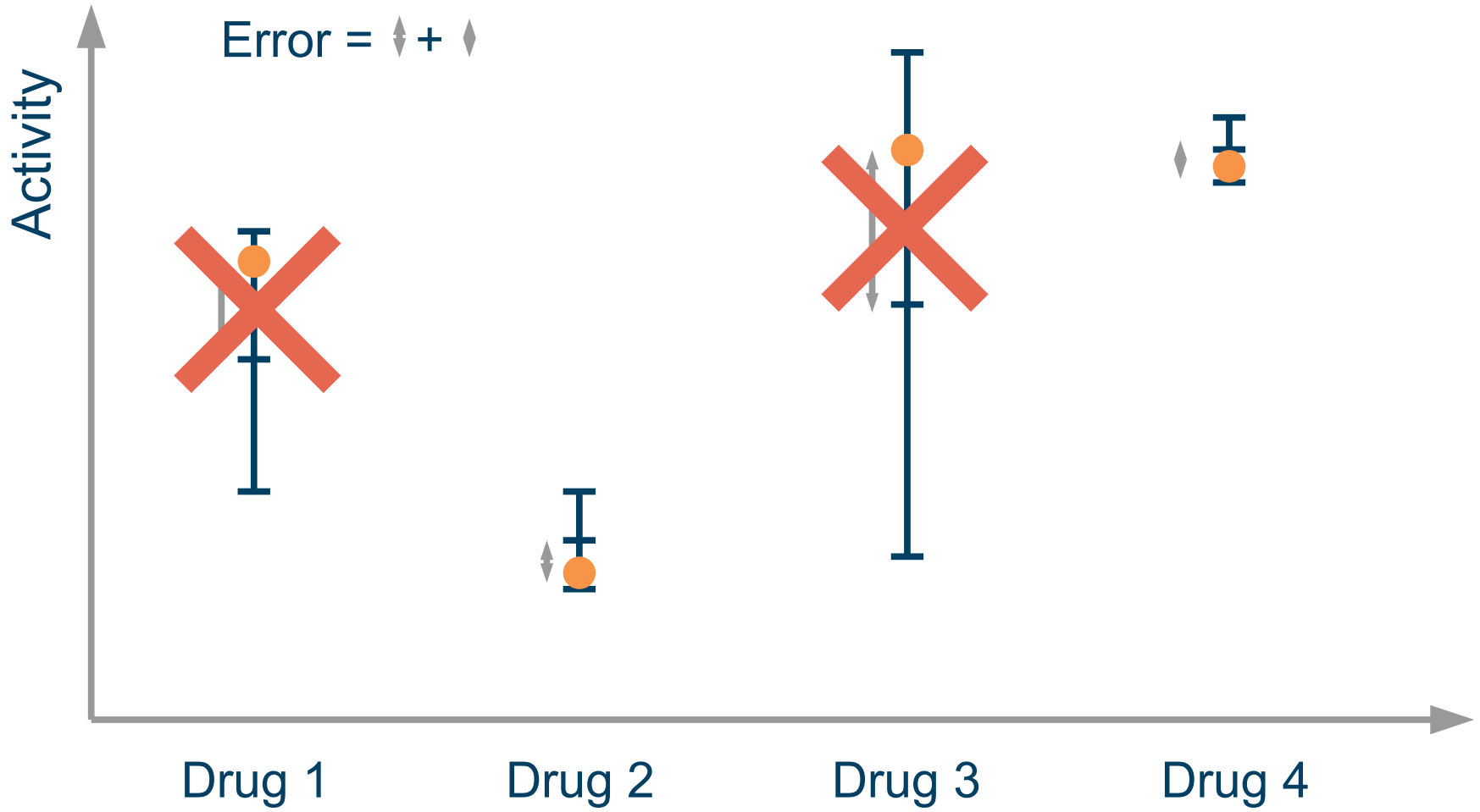
R^2 metric calculated with difference from mean



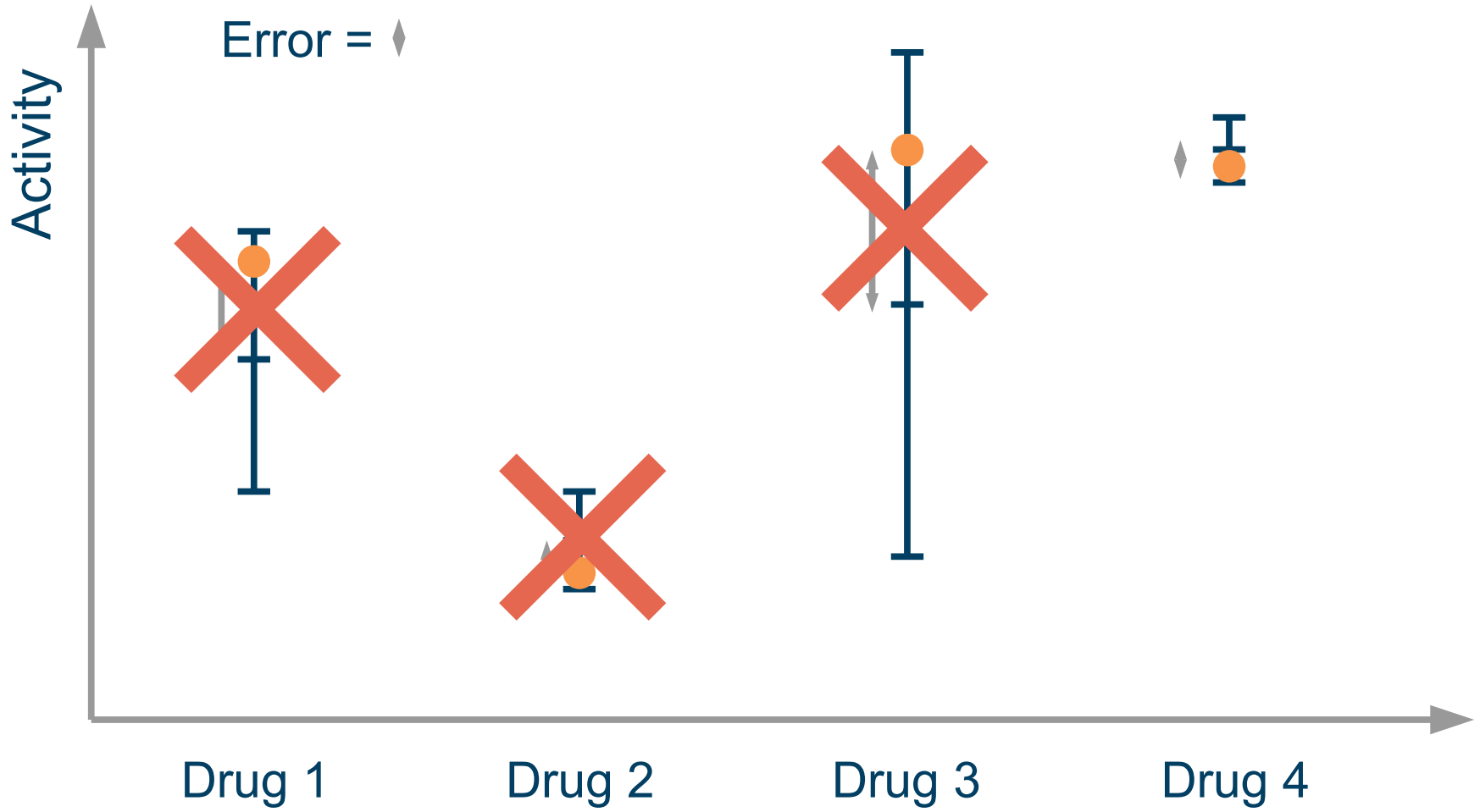
Impute 75% of data with smallest uncertainty



Impute 50% of data with smallest uncertainty



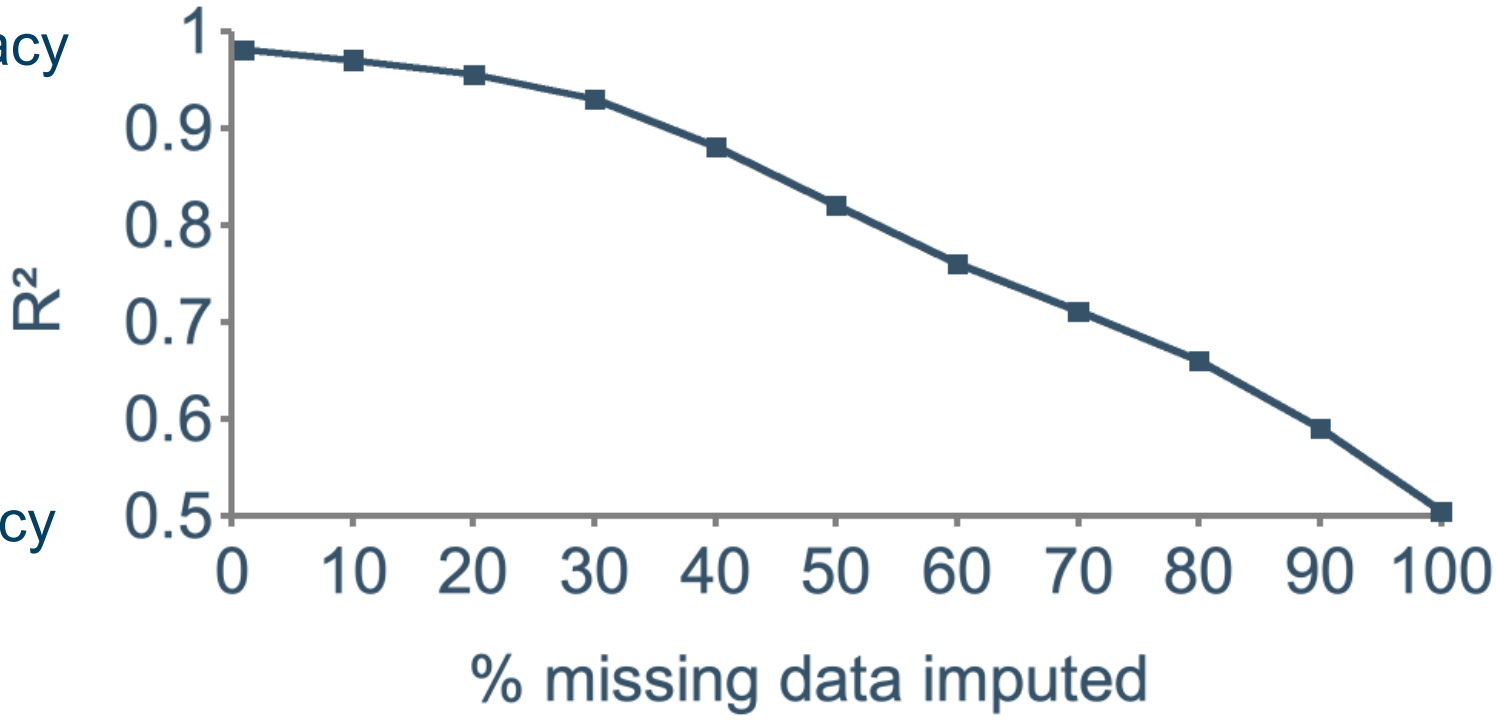
Impute 25% of data with smallest uncertainty



Improved performance by exploiting uncertainty

High accuracy

Low accuracy



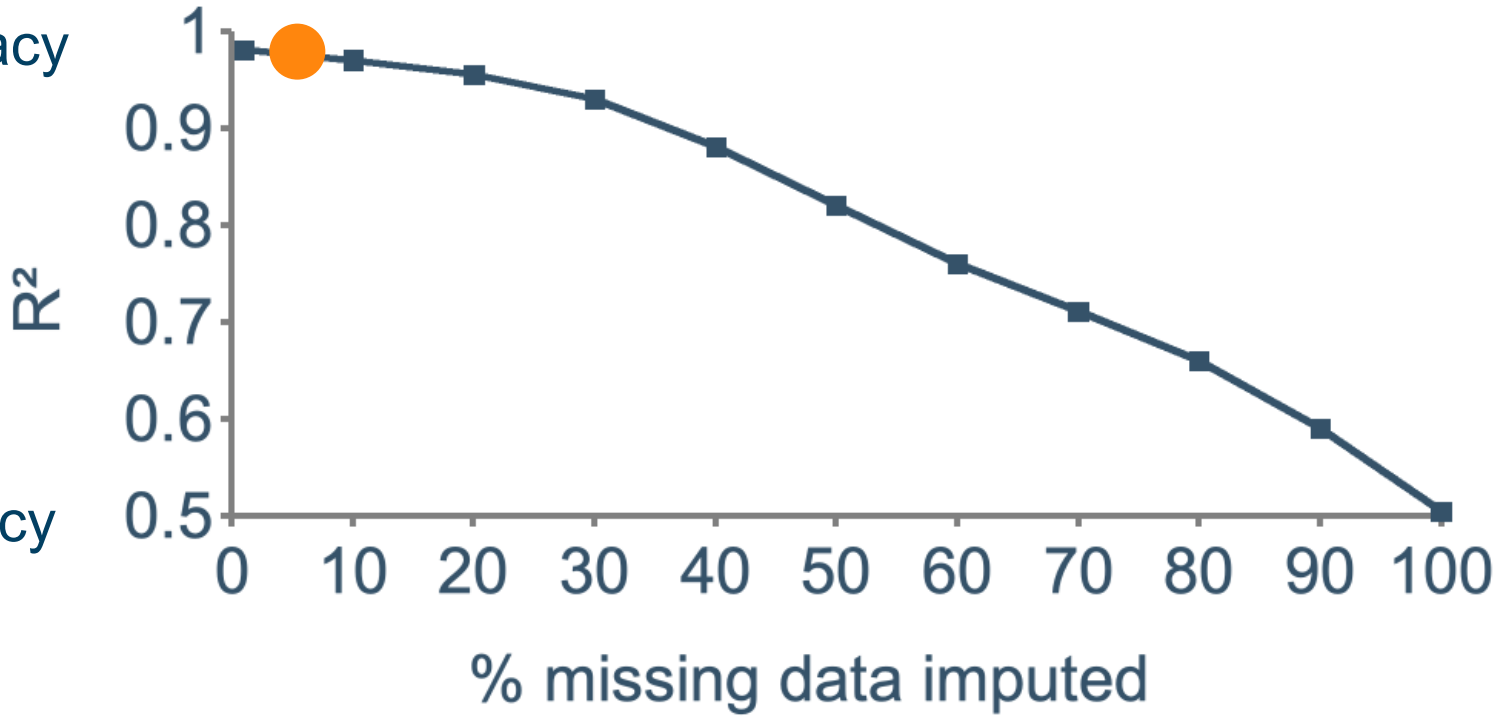
Improved performance by exploiting uncertainty

Different drugs can treat the same ailment

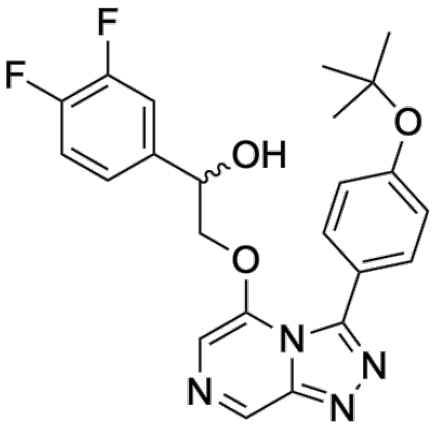
Focus on compounds with low uncertainty

High accuracy

Low accuracy



Open Source Malaria experimental validation



Optibrium & Intellegens

Davy Guan

Exscientia

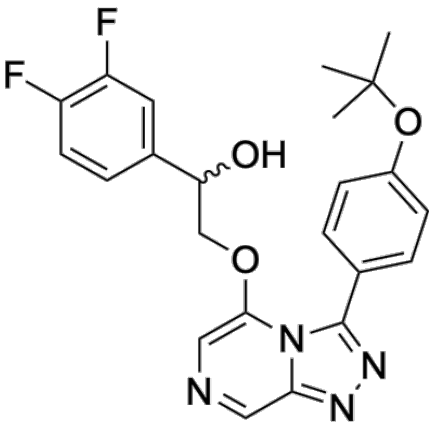
Molomics

0.647 µM

Journal of Medicinal Chemistry **64**, 16450 (2021)

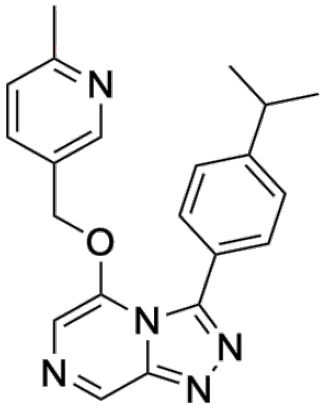
OPEN SOURCE MALARIA
Looking for New Medicines

Open Source Malaria other compounds



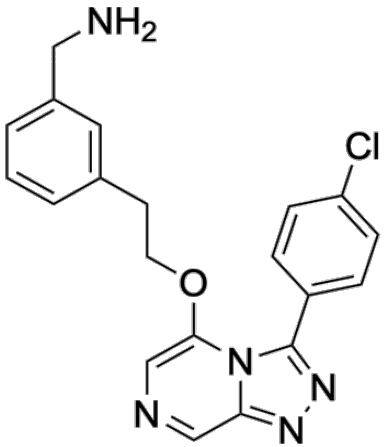
Optibrium & Intellegens

0.647 µM



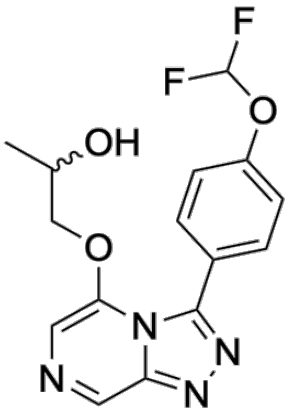
Davy Guan

>25 µM



Exscientia

10.9 µM

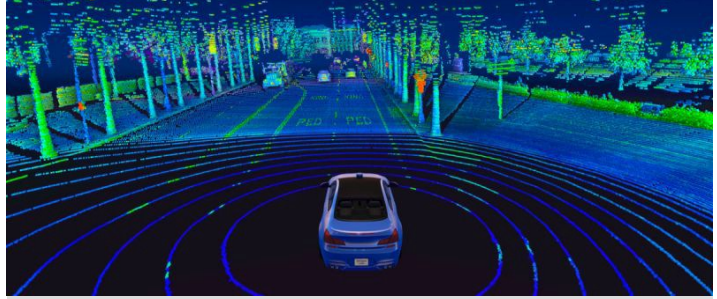


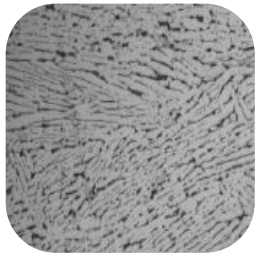
Molomics

>25 µM

Journal of Medicinal Chemistry **64**, 16450 (2021)

OPEN SOURCE MALARIA
Looking for New Medicines





DOMINO

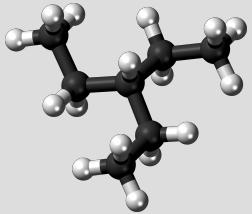
Ordnance Survey

The University Of Sheffield. AMRC Advanced Manufacturing Research Centre

BOEING

GKN

Agency for Science, Technology and Research SINGAPORE



nature machine intelligence

REVIEW ARTICLE

https://doi.org/10.1038/s42256-020-0156-7

Check for updates

Predicting the state of charge and health of batteries using data-driven machine learning

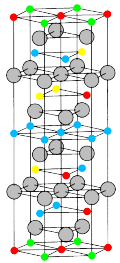
Man-Fai Ng[1], Jin Zhao[2], Qingyu Yan[2]✉, Gareth J. Conduit[3]✉ and Zhi Wei Seh[4]✉

bp

Lubricants
for electric cars

Agency for Science, Technology and Research SINGAPORE

SAMSUNG



NASA

Heat exchanger
& shape memory
alloy applications