intellegens

Applied machine learning

New Products in Less Time:
Fast Experimentation Through Machine Learning

Gareth Conduit

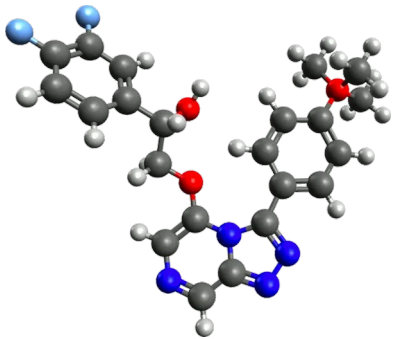
Introduction to machine learning in experimental sciences

Two challenges in the application of machine learning

Case studies for pharmaceuticals and materials

Clinical trials and expensive and time-consuming

Molecule



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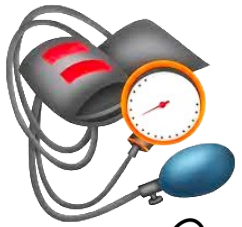
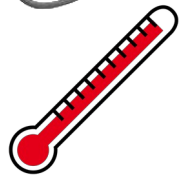
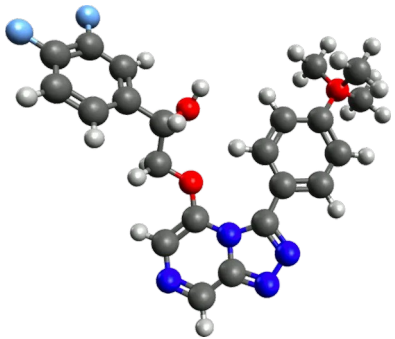
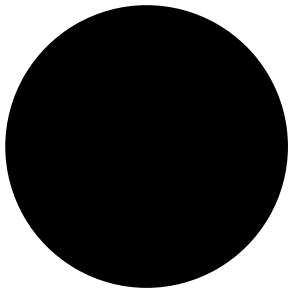




Black box machine learning for drug design

Molecule





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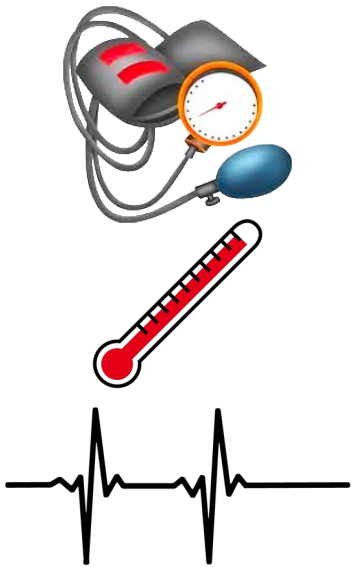
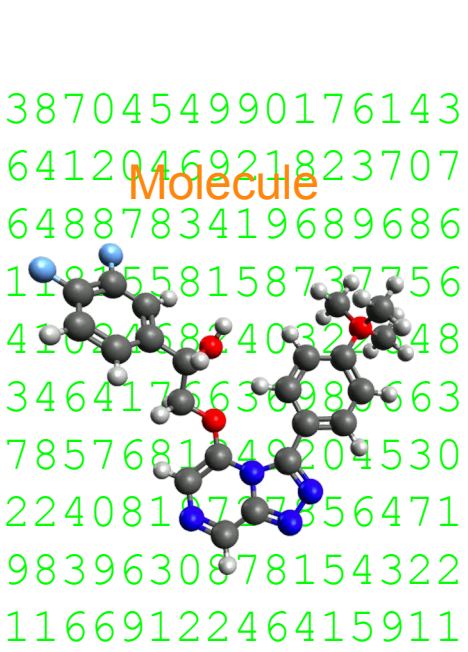
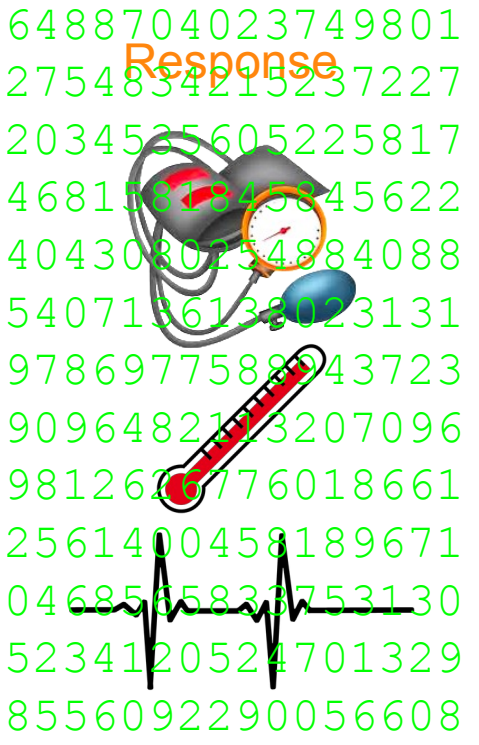


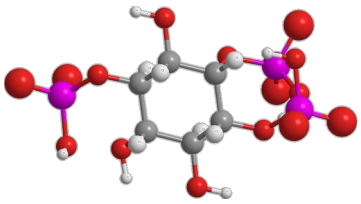
Train the machine learning





Predict behavior of new drug

Molecule



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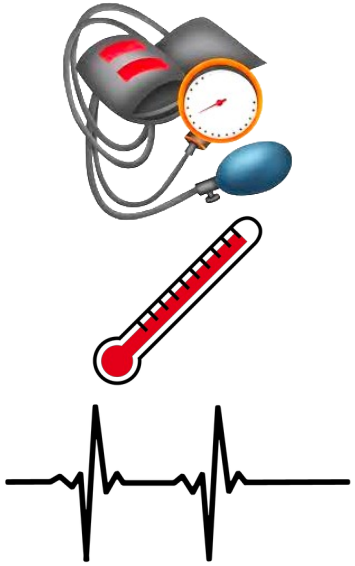
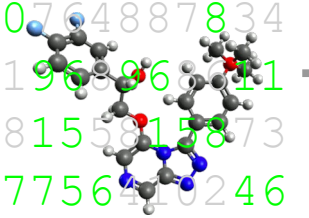


Two challenges in the application of machine learning to practical systems

Sparse data

Molecule



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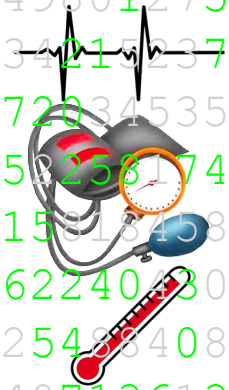
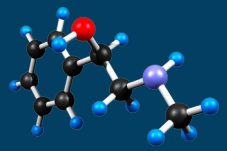
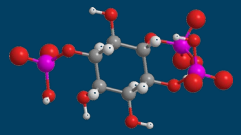
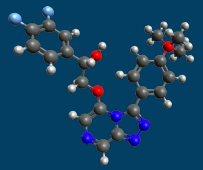
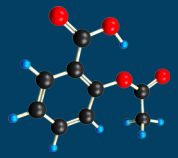
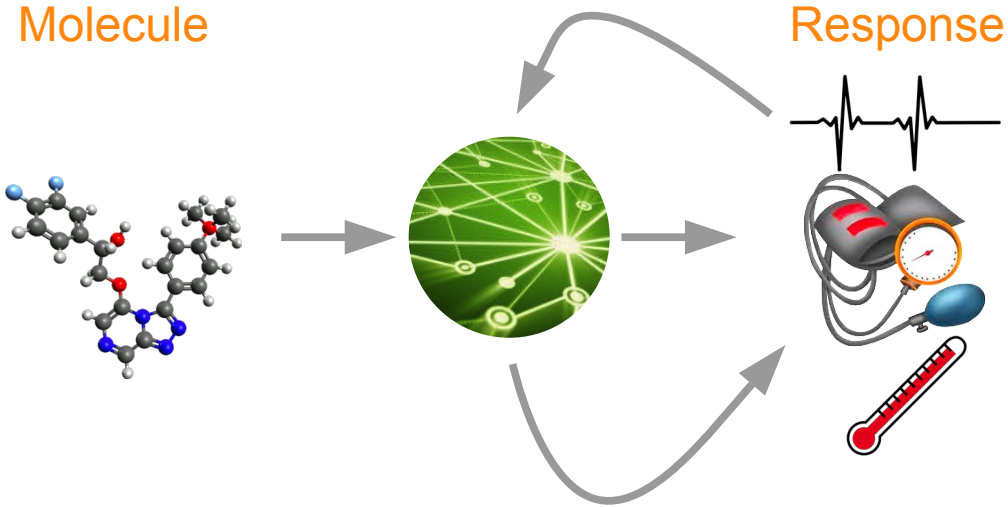


Molecule			
	117 bpm	93 mmHg	36.2 °C
	69 bpm		
	89 bpm	143 mmHg	36.5 °C
		105 mmHg	37.9 °C

Overcome sparsity



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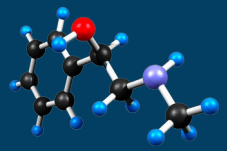
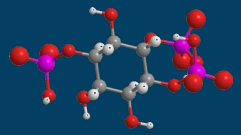
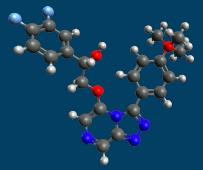
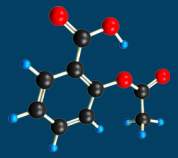
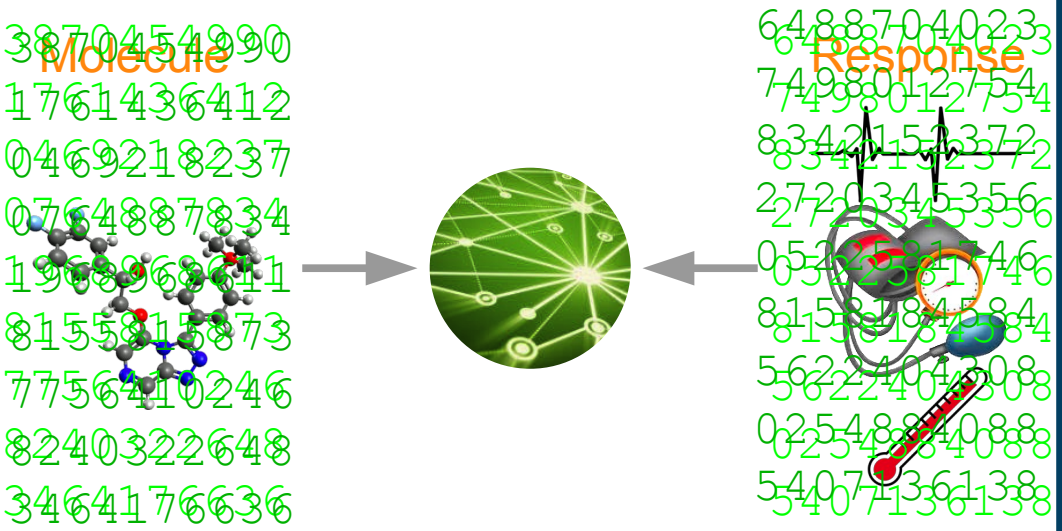
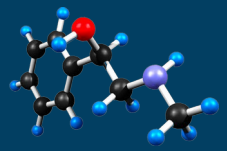
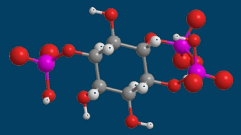
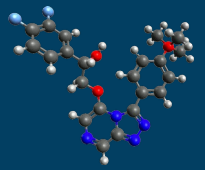
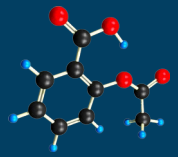
	117 bpm	93 mmHg	36.2 °C
	69 bpm		
	89 bpm	143 mmHg	36.5 °C
		105 mmHg	37.9 °C

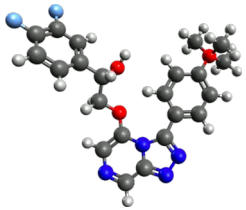
Noisy data



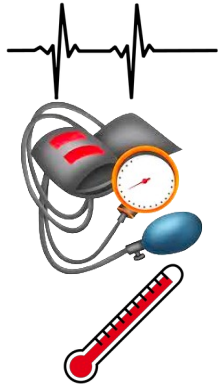
Molecule			
	117 ± 4 bpm	93 ± 7 mmHg	36.2 ± 0.1 °C
	69 ± 2 bpm		
	89 ± 5 bpm	143 ± 2 mmHg	36.5 ± 0.4 °C
		105 ± 8 mmHg	37.9 ± 0.2 °C

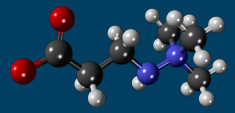
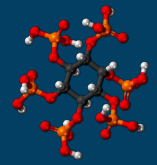
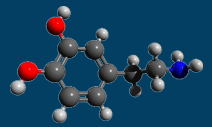
Overcome noise

Molecule



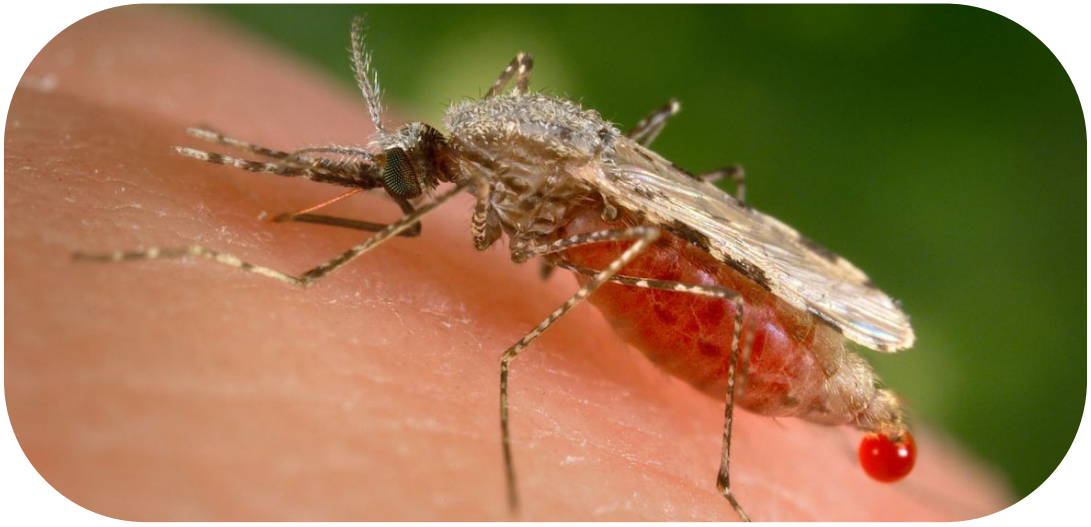
Response



Molecule			
	97 ± 3 bpm	128 ± 3 mmHg	36.6 ± 0.1 °C
	106 ± 7 bpm	91 ± 2 mmHg	36.3 ± 0.4 °C
	116 ± 4 bpm	98 ± 3 mmHg	37.9 ± 0.2 °C
	87 ± 1 bpm	117 ± 7 mmHg	36.8 ± 0.3 °C

Example case studies with Alchemite™

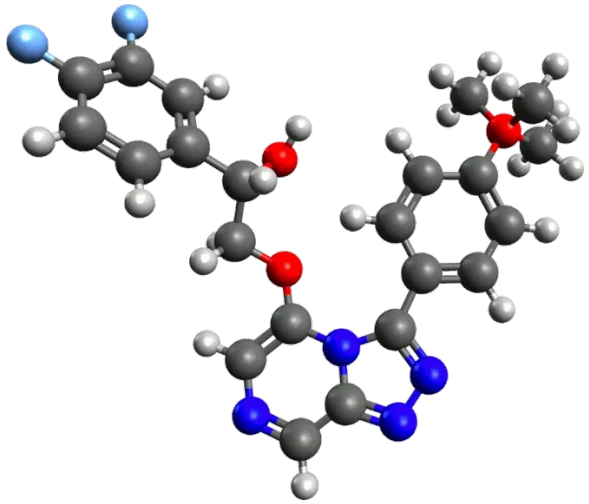
Open Source Malaria contest



OPEN SOURCE MALARIA

Looking for New Medicines

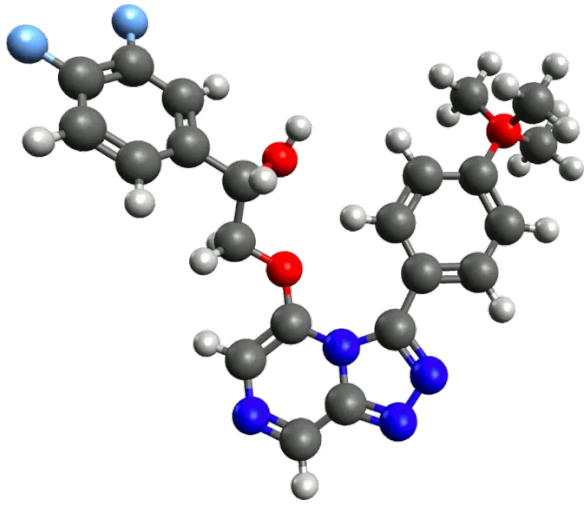
Open Source Malaria competition: winning compound



0.647 µM

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

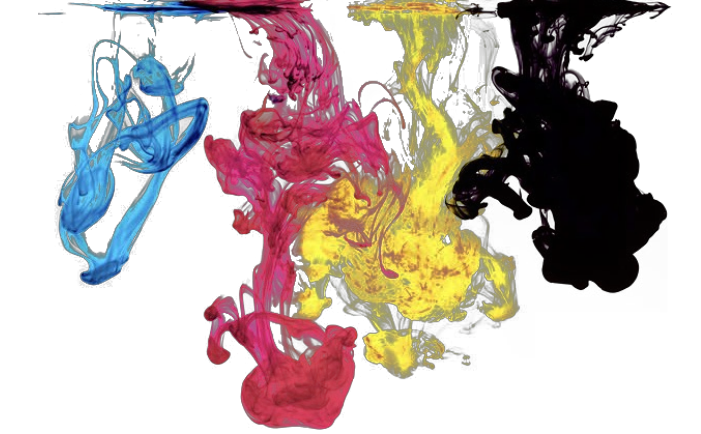
Pharmaceutical partners



0.647 μM

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

Constellation PHARMACEUTICALS
therapeutics
Genentech
A Member of the Roche Group
optibrium
OPEN SOURCE MALARIA
Looking for New Medicines
University of Dundee
Janssen
SANOFI
MILLENNIUM PHARMACEUTICALS, INC
Takeda
Celgene
zoetis
AstraZeneca
Agency for Science, Technology and Research
SINGAPORE



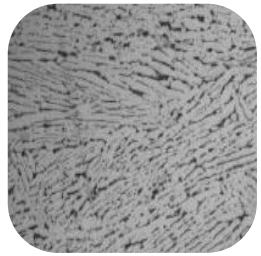
Intellegens
White paper

DOMINO

optibrium

iff

Journal of Computer-Aided
Molecular Design **35**, 1125 (2021)

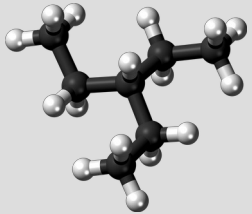


The University Of AMRC Advanced Manufacturing Research Centre

ROLLS ROYCE

NASA

Materials & Design
168, 107644 (2019)



Fluid Phase Equilibria
501, 112259 (2019)
Journal of Chemical Physics
153, 014102 (2020)

bp

nature machine intelligence

REVIEW ARTICLE

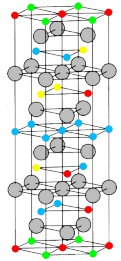
https://doi.org/10.1038/s42256-020-0156-7

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]✉

SAMSUNG



Johnson Matthey
Technology Review
66, 130 (2022)

JM

Machine learning offers significant promise in the applied sciences

Practical issues with noise and sparsity must be overcome with advanced methods

Case studies in materials, chemicals, and drug discovery

Alchemite™ Analytics available through Intellegens

https://intellegens.com

gareth@intellegens.com