intellegens

Research commercialization in Cambridge

Gareth Conduit

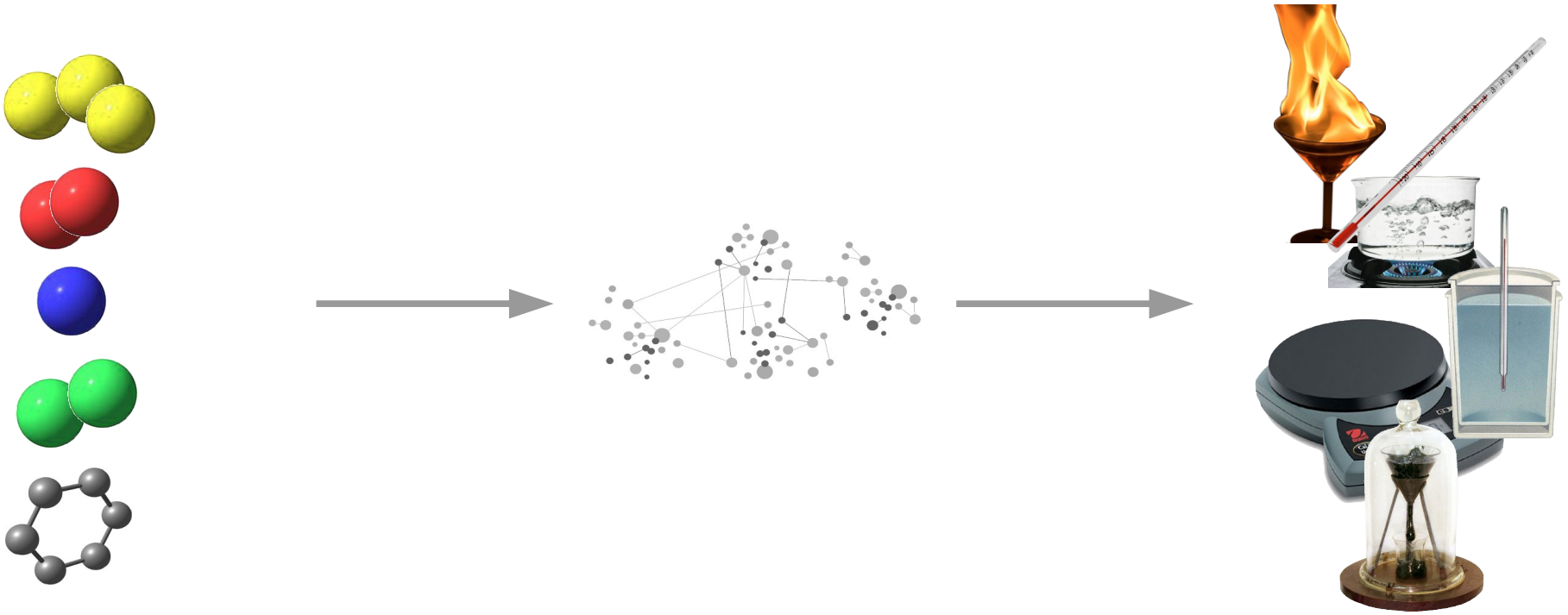
Alchemite™ machine learning tool to

Utilise all available information: computer simulations and real-life measurements

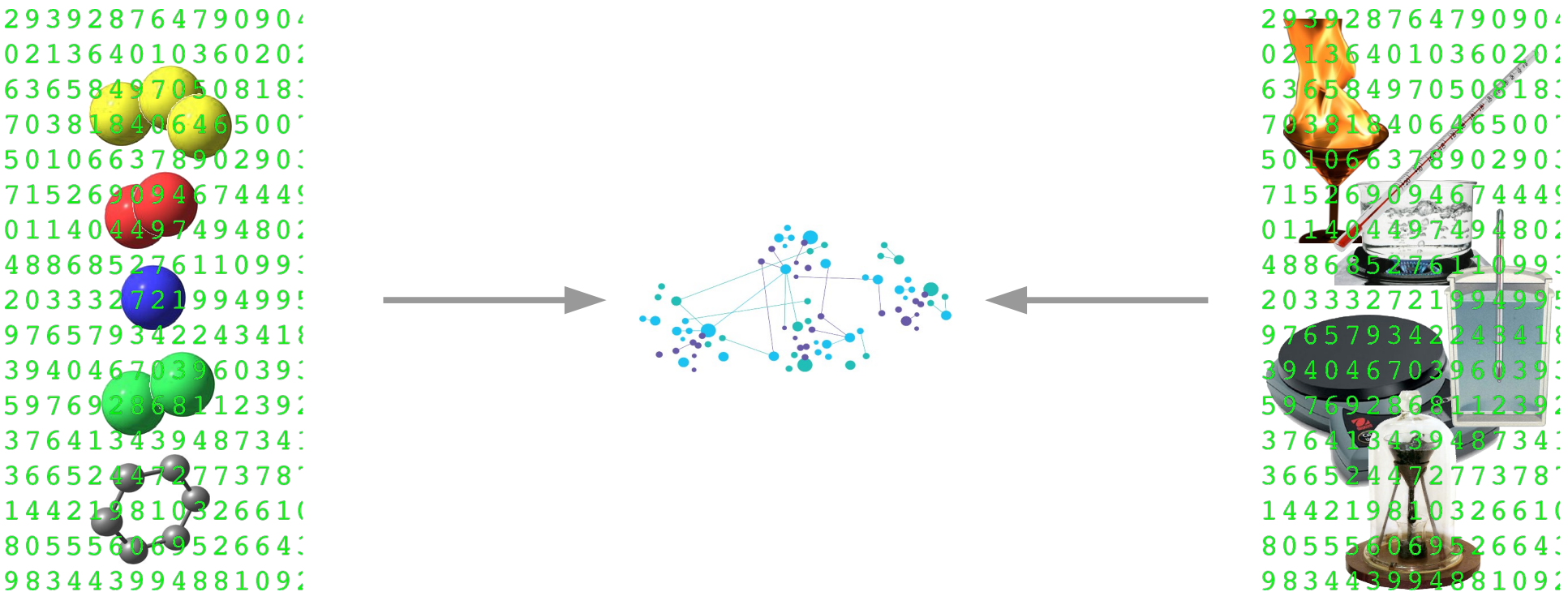
Reduce the need for experiments and accelerate discovery

Broadly applicable with proven applications in drug design, industrial chemicals, and materials

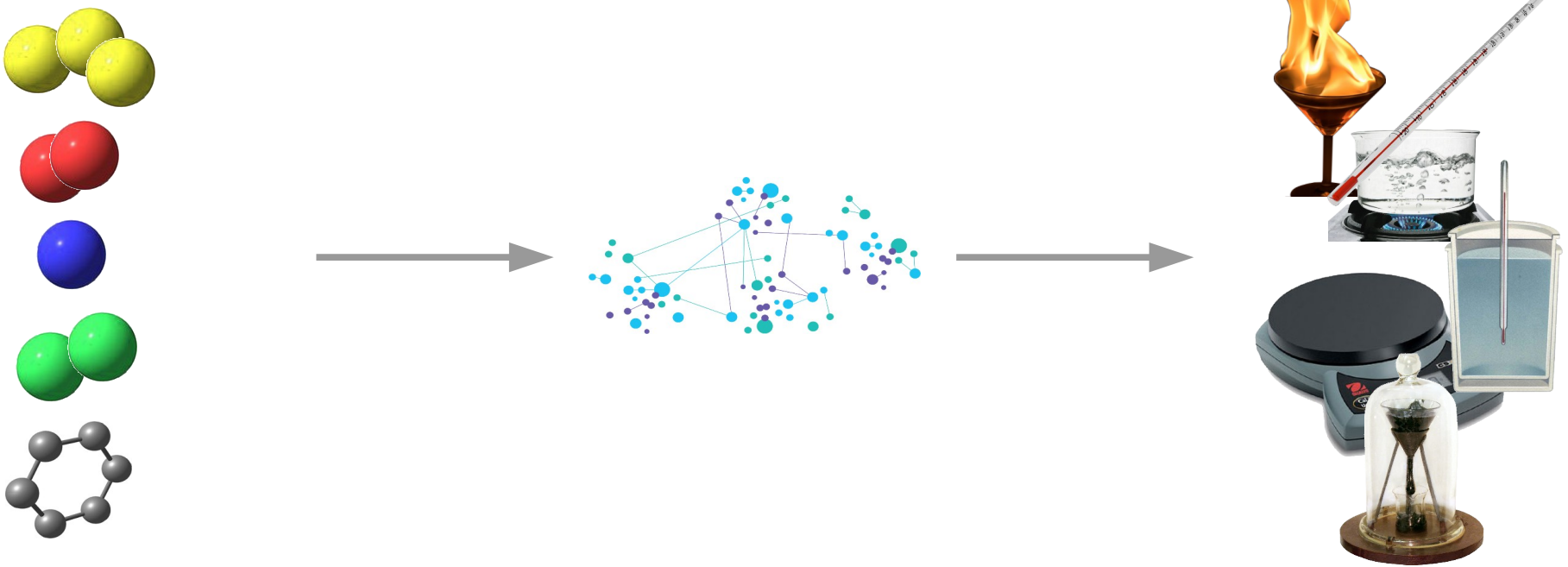
Machine learning as a black box



Train from historical data



Predict new chemicals



First foray into machine learning at University of Cambridge

2013

Multiple properties for Rolls Royce engines

Development of core machine learning ideas

2013	2014
Multiple properties for Rolls Royce engines	Property-property correlations with Rolls Royce and BP

Realign research focus to machine learning

Concurrent materials design

2013	2014	2015
Multiple properties for Rolls Royce engines	Property-property correlations with Rolls Royce and BP	Royal Society University Research Fellowship

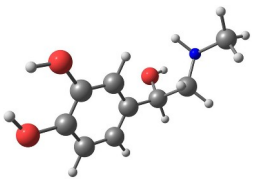
First large machine learning contract as principal investigator

Concurrent materials design

2013	2014	2015	2016
Multiple properties for Rolls Royce engines	Property-property correlations with Rolls Royce and BP	Royal Society University Research Fellowship	Experiment-simulation correlations with Samsung Electronics

Initial application of machine learning to drug discovery

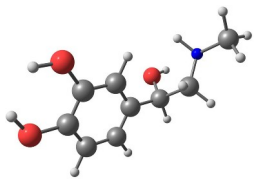
Concurrent materials design



2013	2014	2015	2016	2017
Multiple properties for Rolls Royce engines	Property-property correlations with Rolls Royce and BP	Royal Society University Research Fellowship	Experiment-simulation correlations with Samsung Electronics	Drug discovery study with e-therapeutics

Commercializing the methodology

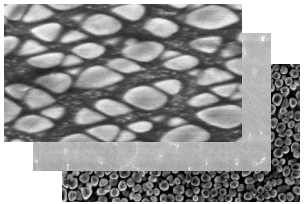
Concurrent materials design



2013	2014	2015	2016	2017	2018
Multiple properties for Rolls Royce engines	Property-property correlations with Rolls Royce and BP	Royal Society University Research Fellowship	Experiment-simulation correlations with Samsung Electronics	Drug discovery study with e-therapeutics	Founding of Intellegens

Materials designed

Nickel and molybdenum



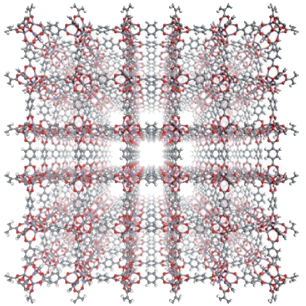
Steel for welding

Experiment and DFT for batteries

More materials designed

Ink formulations

Metal organic framework



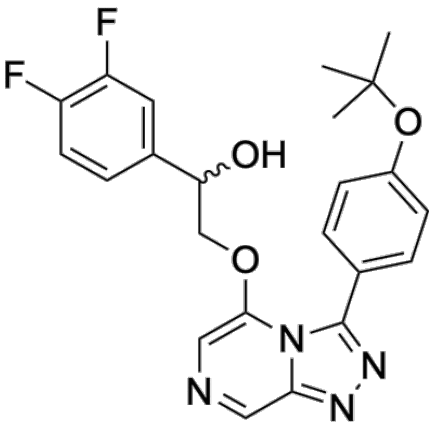
Lubricants with molecular dynamics and experiments

Open Source Malaria competition

OPEN SOURCE MALARIA

Looking for New Medicines

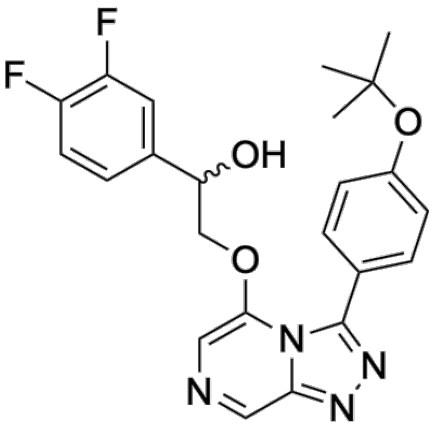
Open Source Malaria experimental validation



Optibrium & Intellegens

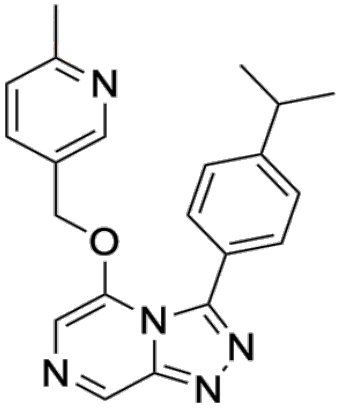
0.647 µM

Open Source Malaria other compounds



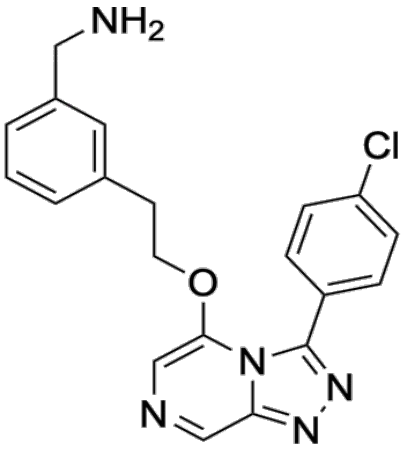
Optibrium & Intellegens

0.647 µM



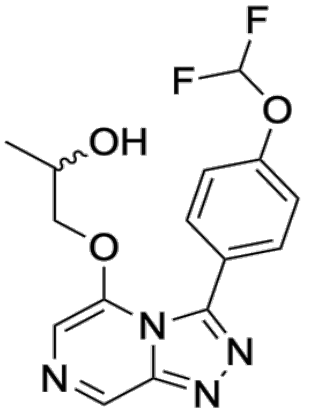
Davy Guan

>25 µM



Exscientia

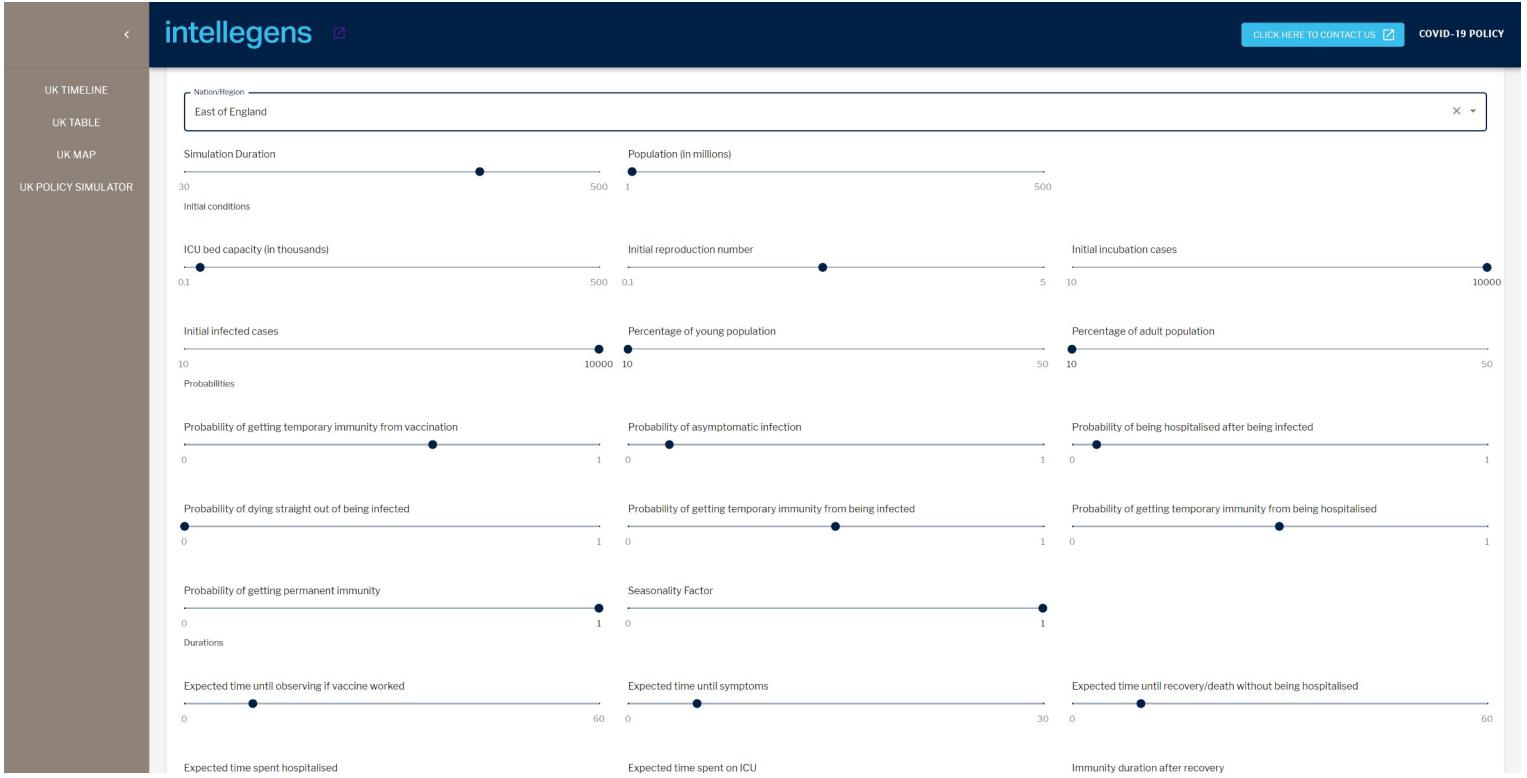
10.9 µM



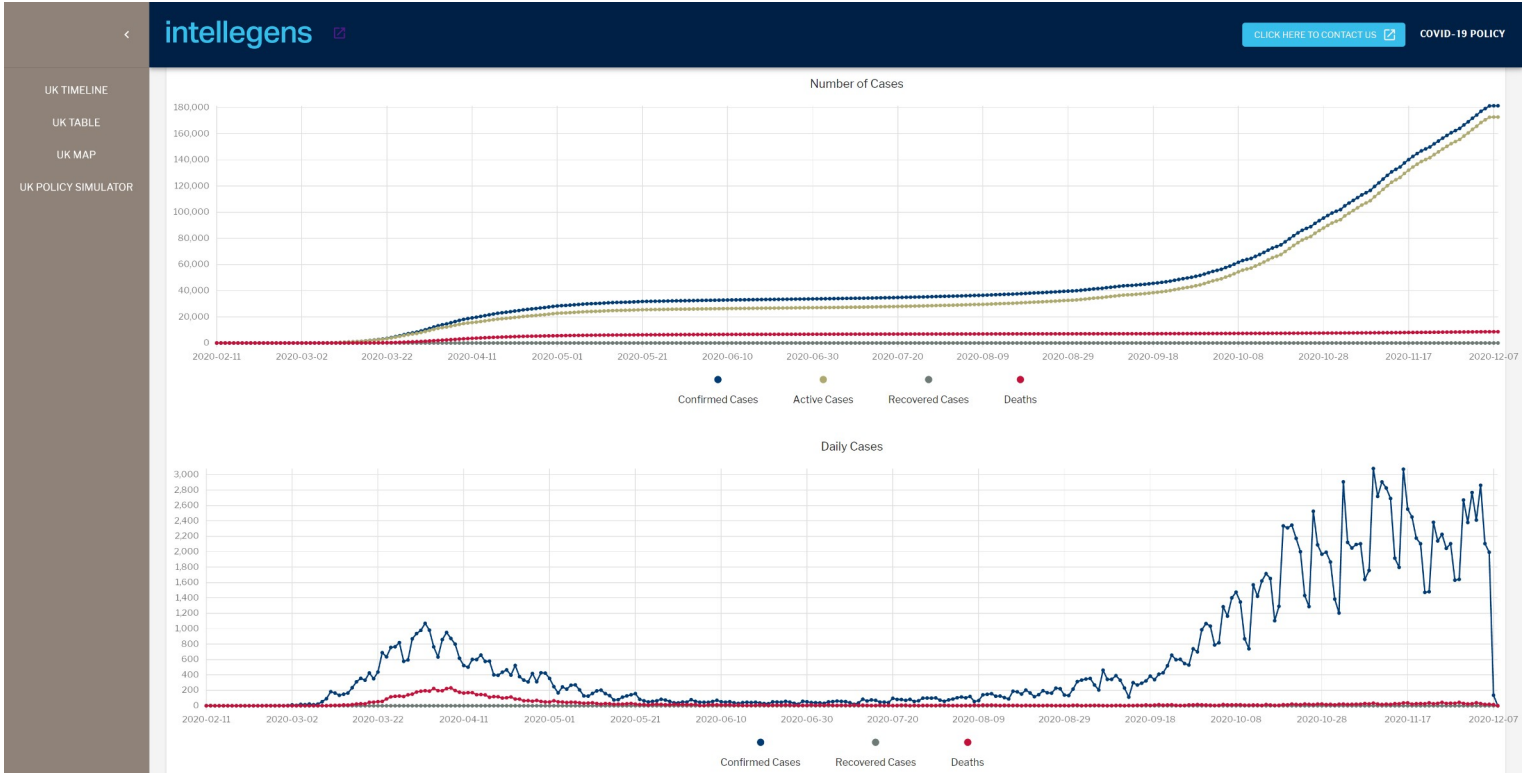
Molomics

>25 µM

COVID-19 modeling: inputs



COVID-19 modeling: outputs



COVID-19 modeling: market

Utilise all available information: daily and weekly information from different countries

Predictive tool for supplier to anticipate market demand

Long-term application to seasonal diseases such as influenza

Initial contracts for Intellegens

therapeutics

2018

Bring across contracts from University

Starting the development of a product

Demonstrator for application of AI to experimental data

2018

Bring across contracts from University

2018

InnovateUK grant

Enter the market as a reseller

therapeutics

Innovate UK

optibrium

Demonstrator for application of AI to experimental data

2018	2018	2018
Bring across contracts from University	InnovateUK grant	Reseller agreement with Optibrium

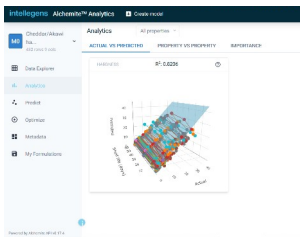
Build out technology through consultancy projects

Demonstrator for application of AI to experimental data

2018	2018	2018	2019
Bring across contracts from University	InnovateUK grant	Reseller agreement with Optibrium	Consultancy work

Launch Intellegens generic industrial formulations product

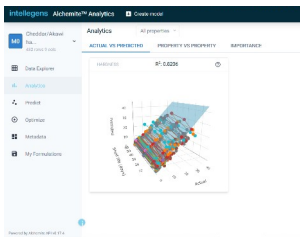
Demonstrator for application of AI to experimental data



2018	2018	2018	2019	2020
Bring across contracts from University	InnovateUK grant	Reseller agreement with Optibrium	Consultancy work	Release Alchemite Analytics™ product

Launch drug design product

Demonstrator for application of AI to experimental data



2018	2018	2018	2019	2020	2021
Bring across contracts from University	InnovateUK grant	Reseller agreement with Optibrium	Consultancy work	Release Alchemite Analytics™ product	Reseller agreement with Ansys

Questions for commercialization of research

Investment	Organic growth or seek venture capital
Breadth	Generic technology, but how many verticals should we enter?
Sales	Enter a vertical directly or through a reseller?
Exit strategy	Seek maximum impact but opportunity to develop next idea

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Papers	https://www.intellegens.ai/paper.html