

# MedChemica

Who are we, What do we do

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## About Us **Passionate about generating better decisions from data**



**Dr Andrew G. Leach**  
Technical Director  
Liverpool John Moores  
12 years experience  
Applied computational  
and medicinal chemistry



**Dr Ali Griffen**  
Business Analyst  
*PhD Fungal Vascular wilt disease*  
21 years experience Team leader  
bioscientist and biological data  
curation



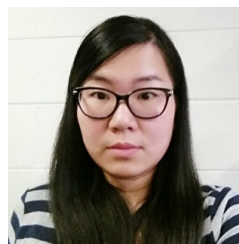
**Dr Ed Griffen**  
Technical Director  
21 years experience  
Medicinal chemistry and  
large scale statistical  
analysis methods



**Dr Al Dossetter**  
Managing Director  
17 years Medicinal chemistry and  
extensive cloud computing  
experience



**Dr Shane Montague**  
Lead Data Scientist  
PhD Computer Science  
13 years experience Data  
science and information  
security



**Dr Jia Wu**  
Consultant Data Scientist  
PhD Machine Learning  
12 years experience in data  
mining and machine learning.  
Projects in finance, energy and  
criminology.

# Collaborators and Users



Medicines for Malaria Venture



BLUEBERRY THERAPEUTICS



THE UNIVERSITY of LIVERPOOL



UNICAM



DUNDEE



WARWICK



MANCHESTER 1824  
The University of Manchester



Liverpool John Moores University

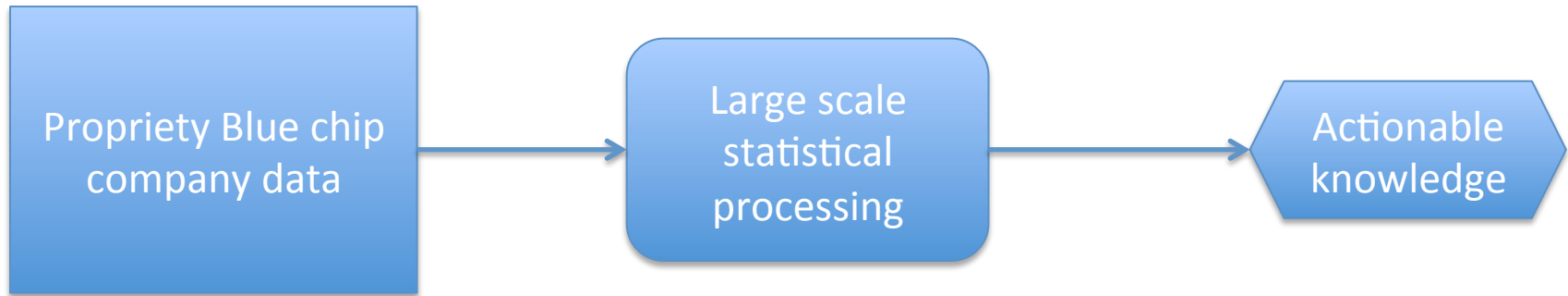


The University of Sheffield.



ICR The Institute of Cancer Research

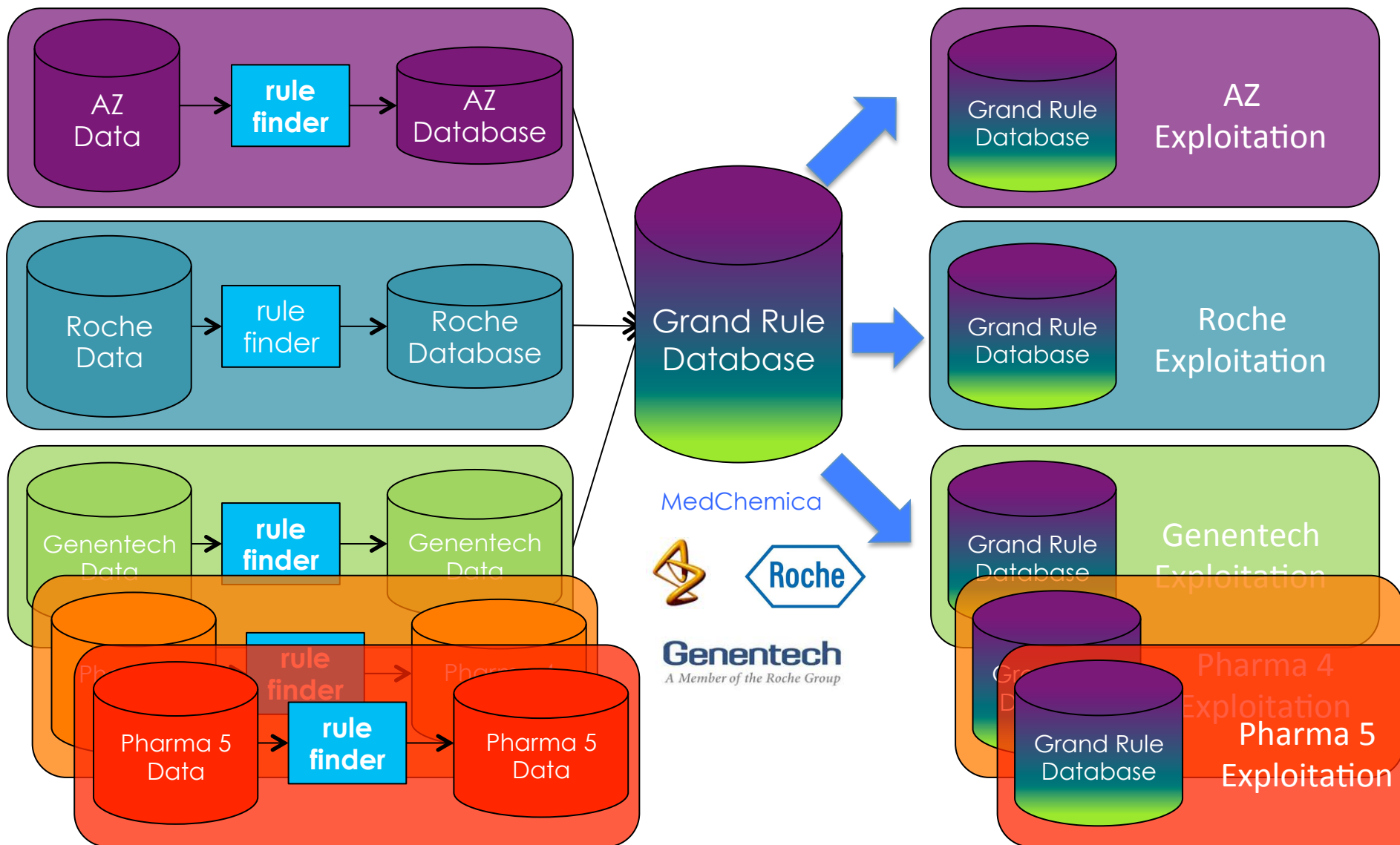
# What we do



- Handle large amounts (>1Tb/year) of company sensitive data
  - **confidentiality**
  - **security**
- Model and analyze complex data types: data complicated by substantial experimental variation, categorical, “censored”
  - **Data cleanliness and validation**
  - **non-parametric statistical methods**
- Apply leading edge computational and statistical methods
  - **scalable cloud solutions**
- Deep understanding of the biological data domain
  - **spot “data supply” issues**
  - **vital to rationalize results – must “make sense”**
  - **relating trends in data with underlying causality**

# Grand Rule database

Better medicinal chemistry by sharing knowledge not data & structures



## Roche, Astra to Share Drug Research Data

**Bloomberg**

### Swiss Stocks Advance on German Confidence Report

#### Roche Partnership

Roche advanced 2 percent to 223.30 Swiss francs. The company struck a partnership with AstraZeneca to share data on early-stage drug design, WSJ reported. Under the agreement, both companies will contribute data to a third company, U.K.-based MedChemica Ltd., WSJ said.

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## MARKETFORCESLIVE BLOG

**theguardian**

### AstraZeneca adds more than 2% on reported R&D tie-up with Roche

Companies said to start sharing data on early stage drugs to help accelerate development of effective medicines

# Technologies and Capabilities

Scalable secure  
infrastructure

Parallel high  
performance  
computing

“Big data”  
databases

Robust  
modern  
statistics

Network  
analysis

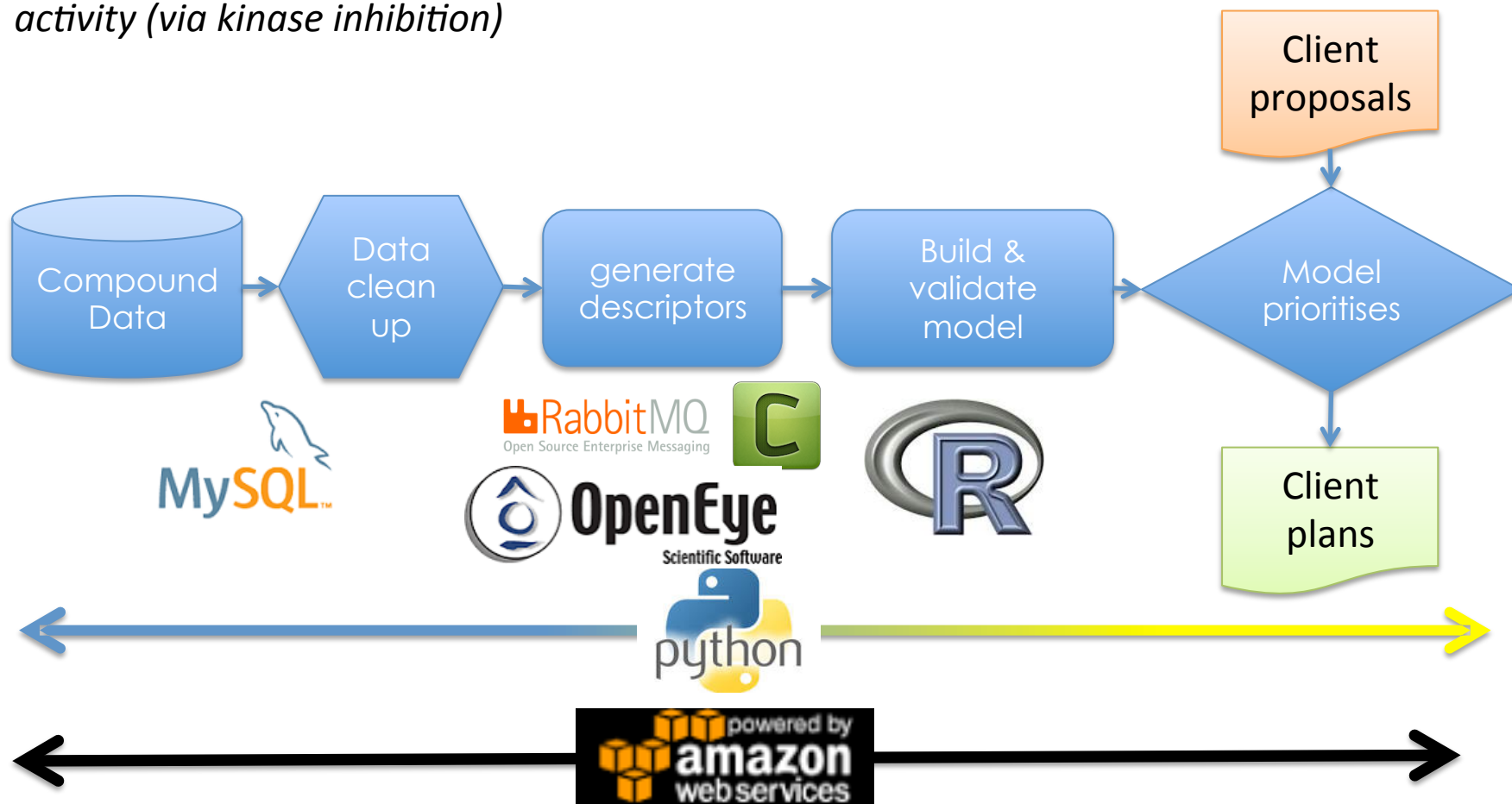


## Analytical approaches

- non parametric linear & non-linear modelling
- matched pair analysis
- neural network analysis
- decision trees
- Bayesian networks
- process mining
- time-series analysis and multi-objective optimisation
- network analysis & graph mining
- clustering

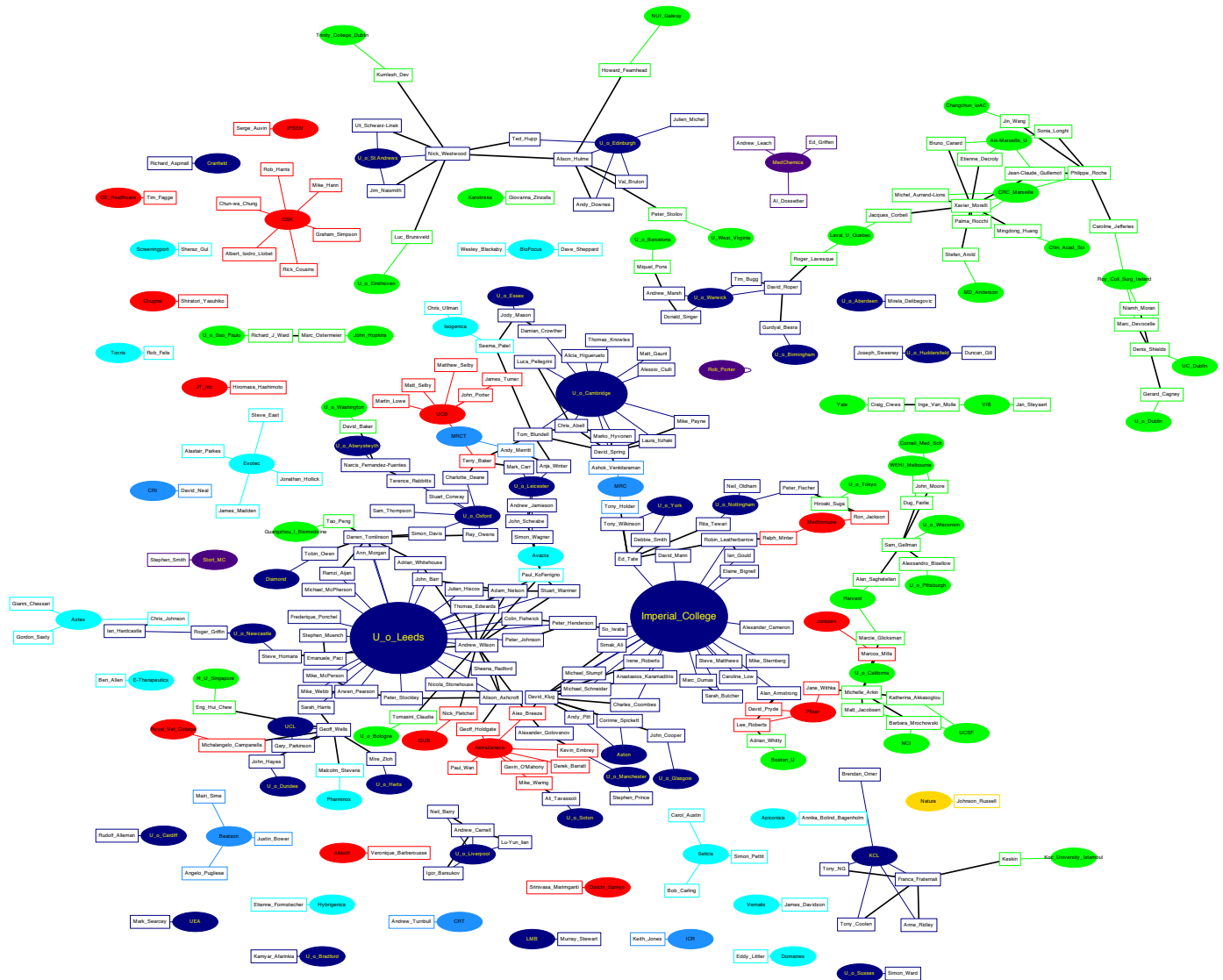
# Better decisions by data analysis

**Client problem:** *how to focus our chemical compound synthesis of compounds we can sell as being more likely to have anti-cancer activity (via kinase inhibition)*





# Understanding complex relationship networks



# Actionable knowledge: key questions

- **What actions** do you want to take from the knowledge you gain?
- **Who** will take them?
- **What's the benefit** to your organisation?