

MedChemica

Who are we, What do we do

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Al Dossetter, Ed Griffen, Andrew Leach, Ali Griffen, Shane Montague,

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



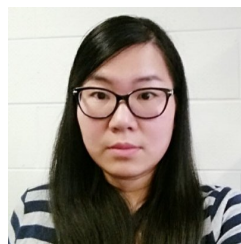
Dr Ed Griffen
Technical Director
21 years experience
Medicinal chemistry and
large scale statistical
analysis methods



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



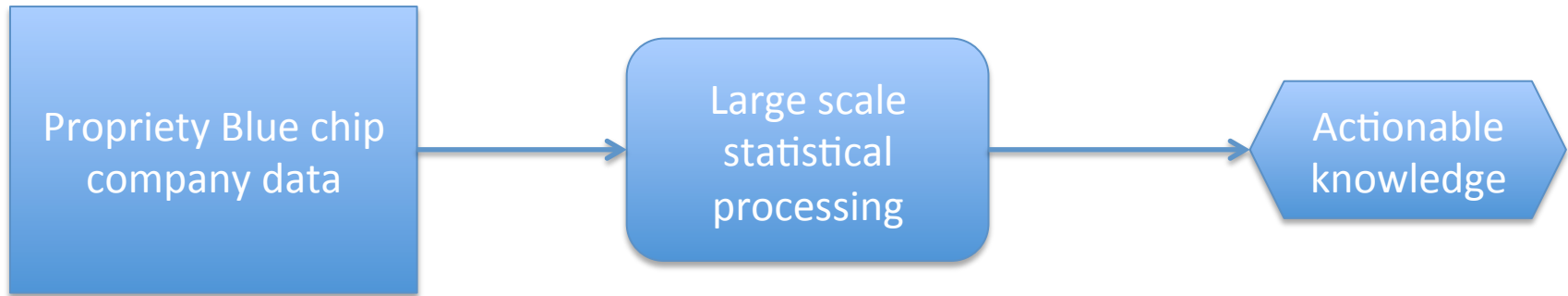
DUNDEE



The University of Sheffield.



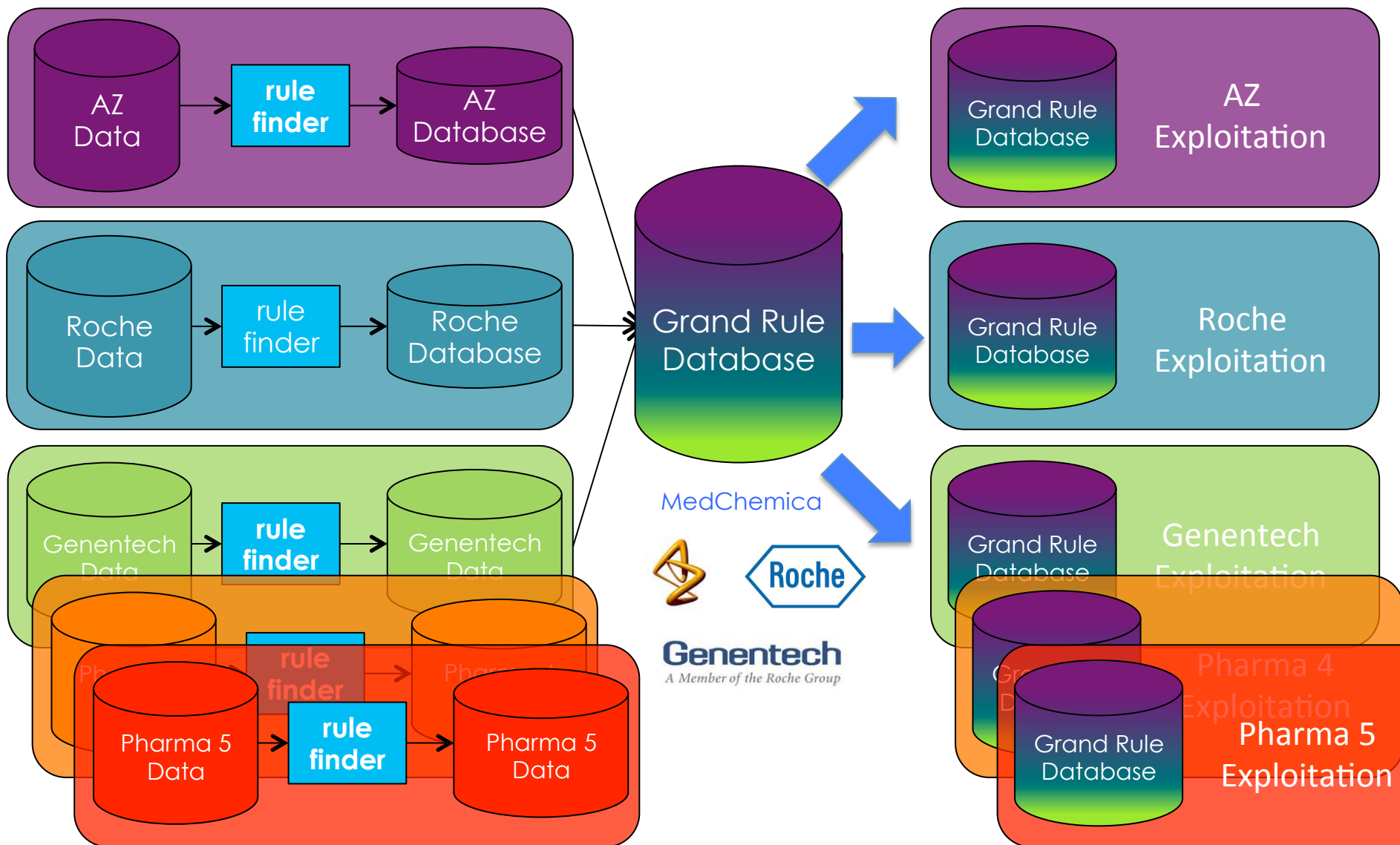
What we do



- 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

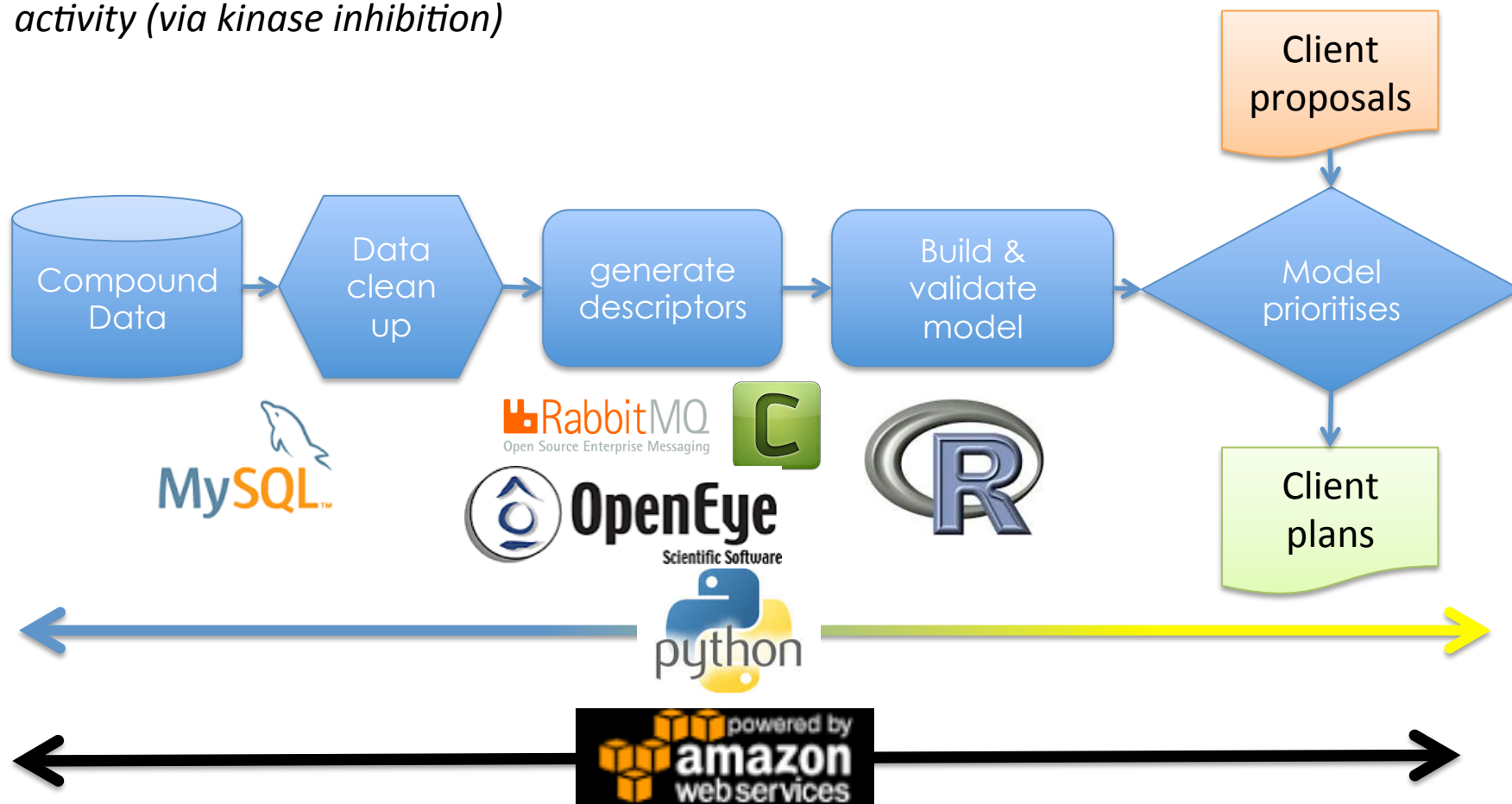


Analytical approaches

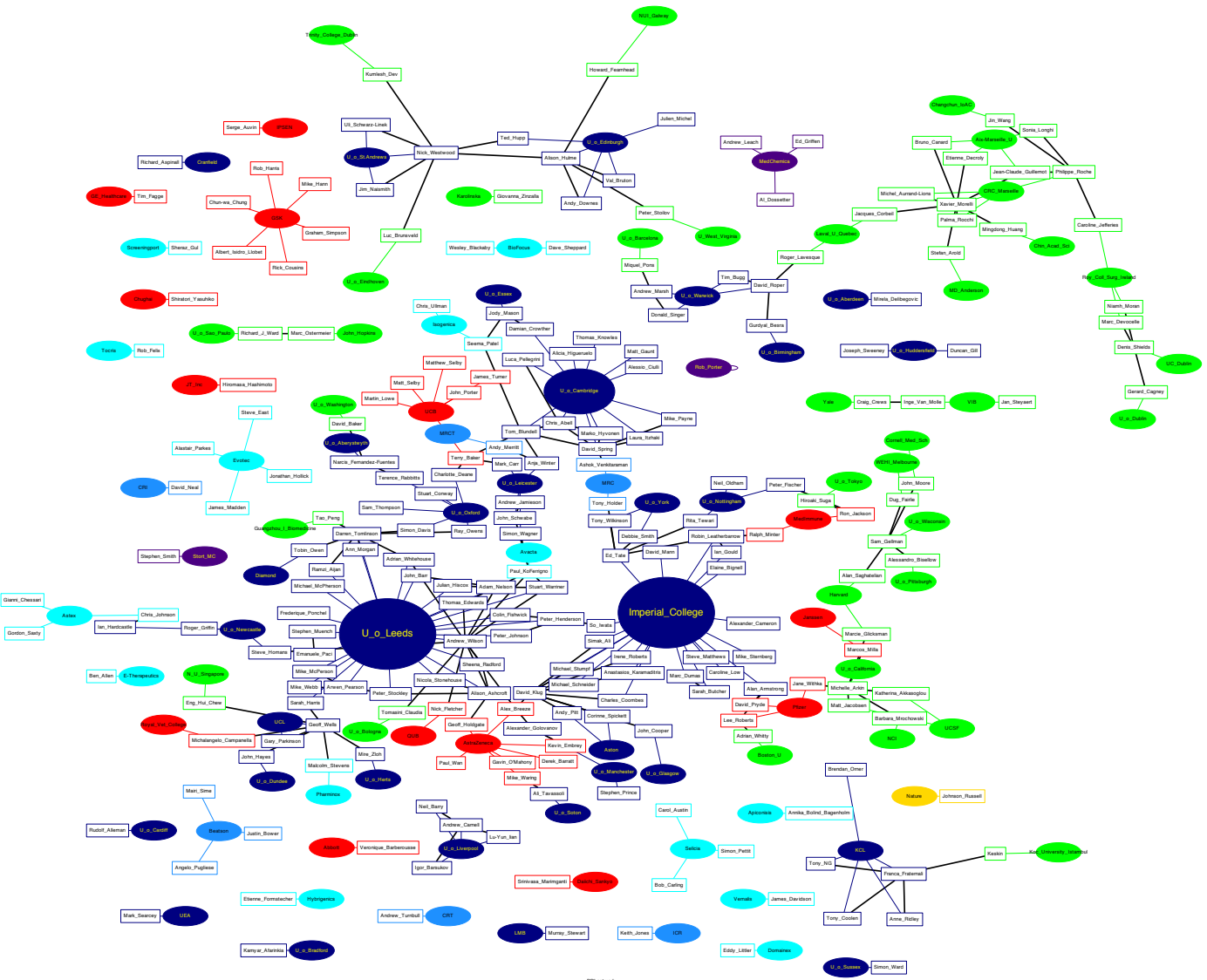
- non parametric linear & non-linear modelling
- matched pair analysis
- neural network analysis
- decision trees
- Bayesian networks
- process mining
- time-series analysis and multi-objective optimisation
- network analysis & graph mining
- clustering

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



PFN network

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?