ChemBio Hub - capturing and sharing chemical biology information and knowhow

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http://chembiohub.ox.ac.uk
Goals of ChemBio Hub

A place to share expertise, equipment, reagents, techniques and current areas of investigation associated with Chemical Biology.

• Improve internal communication
• Improve industry communication
• Encourage investment.
• Re-use/re-cycle pre-existing tools
• Make all available as Open Source
Human PIM1

A protein kinase.

It puts a phosphate on other proteins as a means to cascade important signals within the cell.

When this goes wrong, cancer results.

A small-molecule can help to prevent this by inhibiting the protein’s default action.

But how do we interrogate this?
Generic assay (meta) data capture is very challenging

- There is an incredibly diverse variety of assay data types:
  - qPCR data
  - NMR spectra
  - Phenotypic data
  - IC₅₀ data
  - Western Blot
Challenges for University Researchers

- **Good science**
  i.e. data management

- **Efficiency**
  duplication of effort

- **Fulfilling Grant Conditions**
  open data

- **Personal progression**
  finding effective collaborators

- **Outcomes**
  partnerships with industry to bridge the gap
We approached chemists and biologists direct and asked them about:

What they were using to store data (if anything)
What they disliked about their software
Whether sharing data was something they currently did

Lots don’t use anything at all - paper and pen and filed in a “database”...

Sharing was not widespread but scientists could see the benefit
Searching and better data processing were high priorities
Hasn’t this already been fixed?

Sure, there are lots of tools available.
The solution – ChemBio Hub

Capture data, reagents/compounds, expertise –
• With assistance and curation
• In a central repository

Controlled levels of access –
• Within group, department, Oxford or externally

Example outcomes:
• The ‘go-to’ location for all aspects of University Chemical Biology
• Ability to discover tool compounds against target/protein of interest
• Identification of possible translational routes
• Pushing data externally, attracting pharma funding towards novel targets
Not just for chemistry...
Example Alpha Screen data flow

- Raw input
- Reshaping
- Dose-response curve fitting + Data cleansing
- Saved to ELN
The solution: ChemBio Crunch

1) Upload raw data
2) Validate plates for systematic errors
3) Calculate IC\textsubscript{50} for multiple plates
4) Mark poor fits where observed
5) Export and deposit in ELN (Comments automatically generated where IC\textsubscript{50} may be inaccurate)
The technology stack

What you see
- jQuery
- HTML
- CSS
- Bootstrap
- AngularJS

What that runs on
- Tastypie
- Django
- Gunicorn
- WebAuth
- Apache
- PostgreSQL

What we use to deploy and test it
- GitHub
- Sentry
- Travis CI
- Behave
- Jekyll
- Fabric
Who would use it?

Anyone who manages an inventory through a spreadsheet

- Compounds
- Antibodies
- Cells
- Plasmids
- Lab orders
- Mice
- Unicorns
Why use it?

– Online
– Easy to use
– Search for things instantly
– Reduce duplication
– Free

– Academic project
– Evolving project
– Me!
Weaknesses of an evolving project

– Innate resistance to IT solutions
– System not quite up to scratch
– Unclear message
– Concerns about future
– Group engagement
Advantages of a data management system

For the PI -

Avoid the Post-Doc leaving panic

At the Bench -

Quickly search your data

Across the Department -

Save money – Sharing of resources can reduce departmental spending
Engaged with 80+ labs across 10 departments:

- Chemistry
- Dunn school
- WIMM
- Pharmacology
- DPAG
- Plant Sciences
- Zoology
- Biochemistry
- Oncology
- TDI / SGC
Engagement tools

- Emails / phone calls etc.
- Friends of friends
- ‘Dropping in’
- Departmental meetings
- ChemBio Hub symposium
- Trade stands
Engagement over time

Labs engaged with by Department (June 2016)

No. of Labs

Chemistry | DPAG | Dunn | NDCN | NDM | Oncology | Pathology | Pharmacology | WIIM | Zoology | Plant Sciences

Department
Engagement over time

State of engagement with lab groups (May 2016)

- In production

Number of labs

Group engagement status

- Feb
- May
ChemiReg is in demand

- Clear systemic need for an Inventory manager
- People don’t realise they have a problem
- IT support is not working as it should
- People bemused by computers
Clear University requirement for IT solutions

- Dunn School of Pathology stores inventory
- Chemistry departmental reagent inventory
- Chemistry Mass spec compound registration system
- Plasmid database system
Implementing change – Things to look out for

• Politics

• Novel solutions require an open mind

• Who is the lab authority?

• Lab morale can play a key factor
Things to keep on top of:

• Managing expectations is key

• You can’t please everyone

• User aftercare

• Herding cats
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