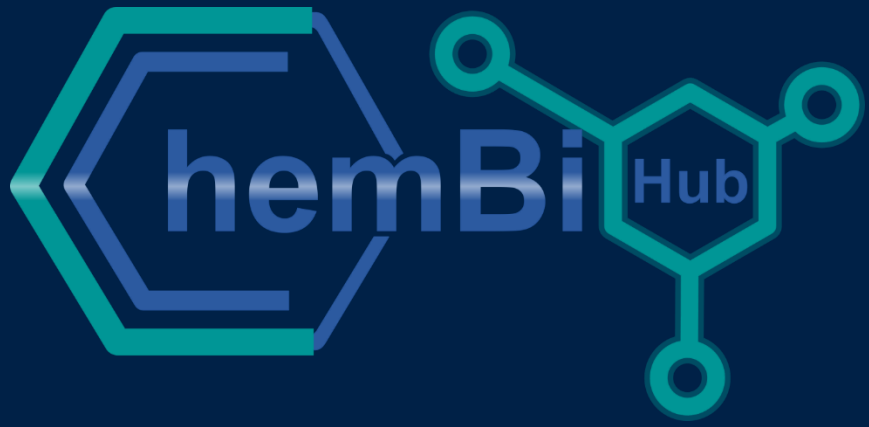
Things to do with Data:

# Taming University Chemical Biology Knowledge




http://chembiohub.ox.ac.uk

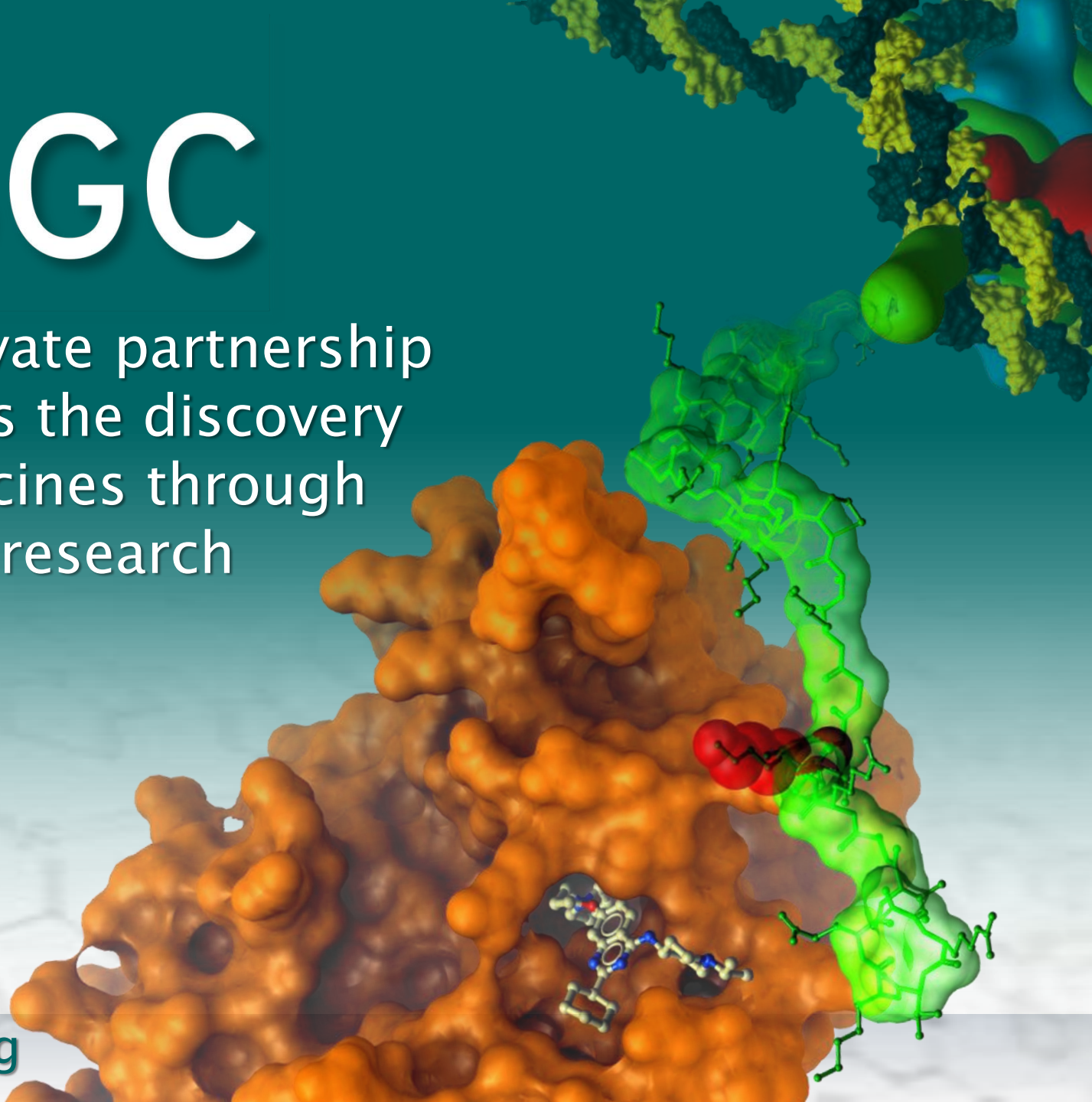
Brian Marsden
SGC, NDM
Kennedy Institute of Rheumatology, NDORMS

## Covering:

- Who am I and why am I here?
- Chemical Biology – what's that?
- The basic science (in 10 minutes)
- So, what's the problem?
- How are we tackling it?
- What have we done so far?
- What's next?

# SGC

A public-private partnership that supports the discovery of new medicines through open access research

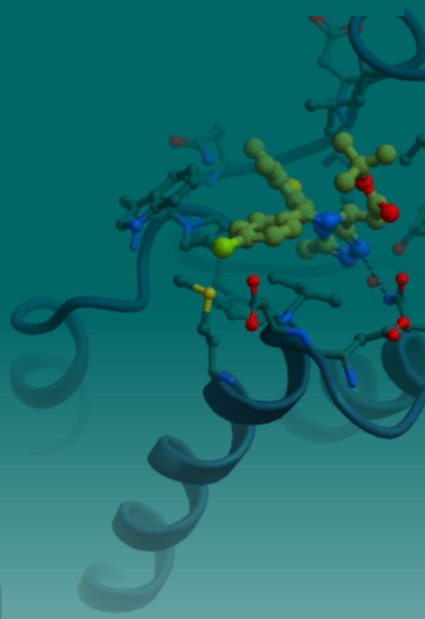


UNIVERSITY OF OXFORD

www.thesgc.org

# SGC at a glance

- Operations started in June 2004
- 3 government agencies, Wellcome Trust and 10 leading pharma companies
- Aggregate funding in excess of $300M
- +200*-strong team in Oxford, Toronto & Campinas
- Open Access Policy:
  - **Promptly placing results, reagents and know-how in the public domain**
  - **SGC scientists never file patents**



wellcome trust Strategic Award · FAPESP São Paulo Research Foundation · gsk GlaxoSmithKline · Novartis · Pfizer · Lilly · Genome Canada · Ontario · Takeda · abbvie · janssen · Boehringer Ingelheim · Bayer

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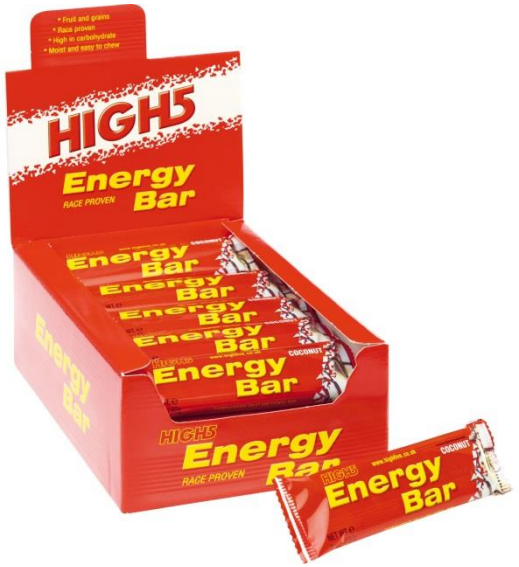
# What is chemical biology?

- Chemical biology means different things to different people

- Are the projects below examples of chemical biology…?

- Designing molecules to act as high-energy foodstuffs



# What is chemical biology?

- Chemical biology means different things to different people

- Are the projects below examples of chemical biology…?

- Using nature's chemistry to produce clean energy

# What is chemical biology?

- Chemical biology means different things to different people

- Are the projects below examples of chemical biology…?

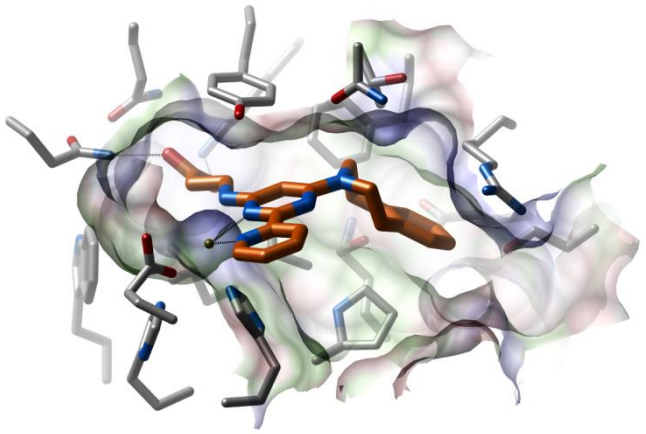
- Tweaking biological structures at the atomic level

# What is chemical biology?

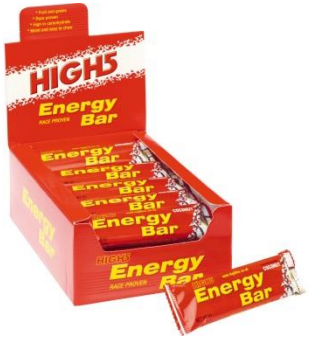
- Chemical biology means different things to different people

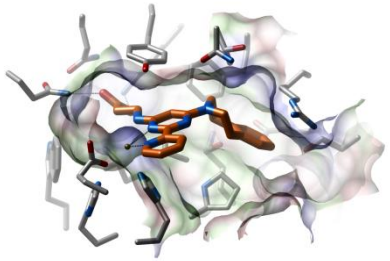
- Are the projects below examples of chemical biology…?

- Testing the effect of chemicals on biological molecules and cells



# What is chemical biology?



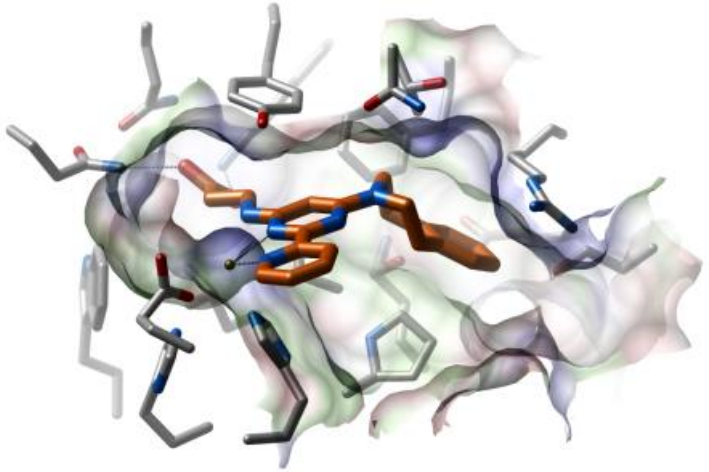



- All these (and more!) can be considered as chemical biology…

  …but also as medicine, physics, engineering, nanotechnology, drug discovery, synthetic biology, biochemistry, etc…

- Too diverse to deal with all at once!

# What *sort* of chemical biology?



- ChemBio Hub initial focus:
  - Effect of chemicals on biological molecules and cells
- Why?
  - Expertise of our group
  - Significant amounts of data generated across the University
  - Demand from pharmaceutical industry for this data
  - Complements public data curation initiatives

    e.g. ChEMBL, PubChem

# And now for the Science 'Bit'...

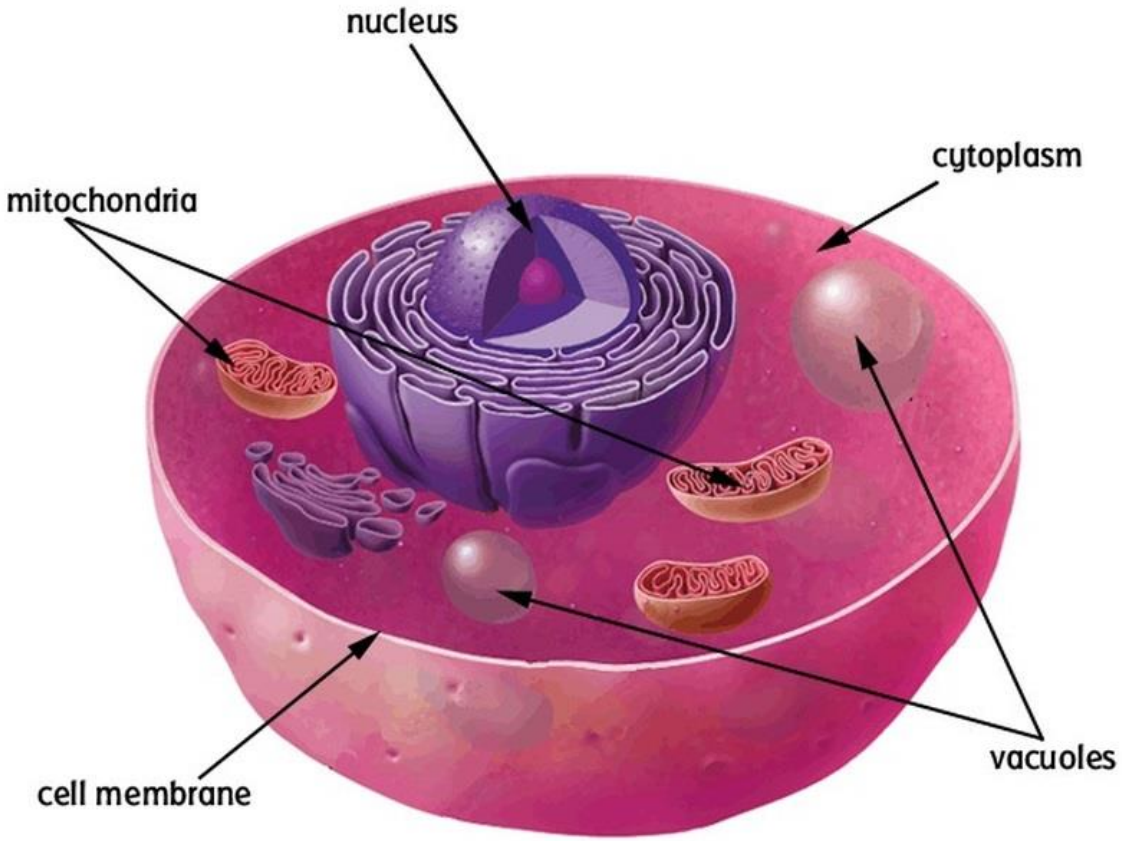
# Cells

The basic unit of living things

Over 200 distinct cell types

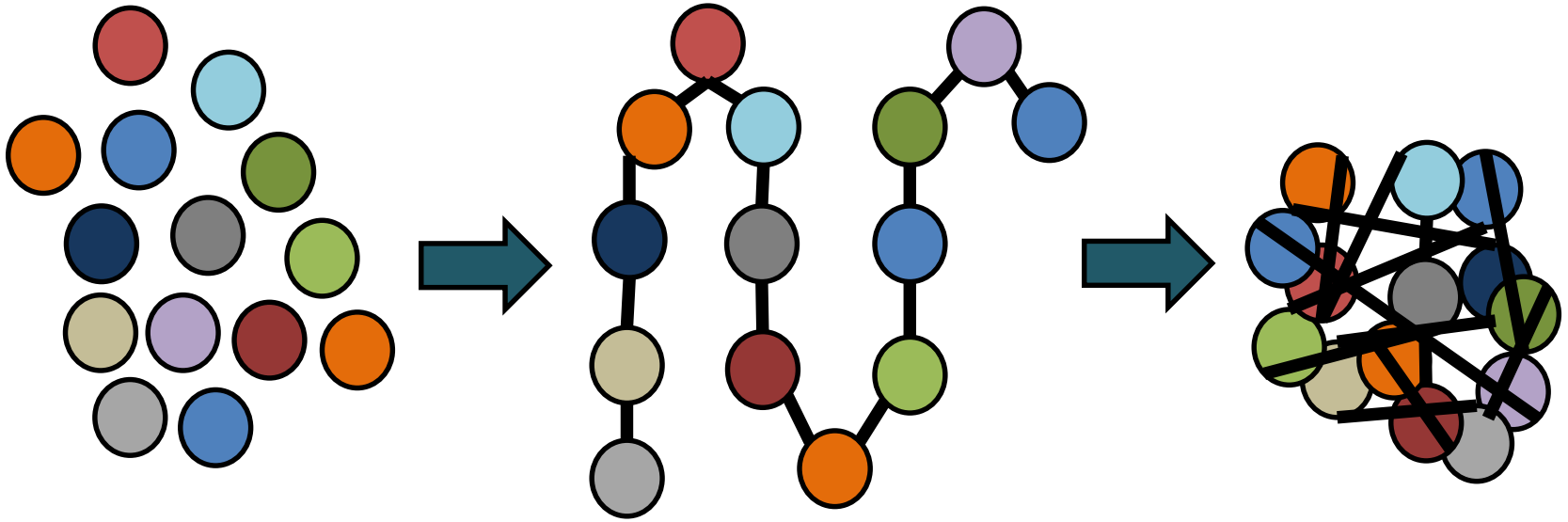
Core components include

- Nucleus
- Mitochondria
- Cytoplasm
- Cell membrane
- Millions of proteins



# What is a protein?

**Proteins** – Large biological molecules consisting of one or more long chains of amino acid residues



Amino Acids:

Proteins are made up individual building blocks

Polypeptide:

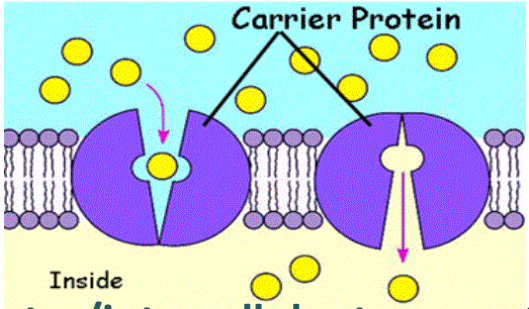
When assembled they form a peptide chain

Protein:

Specific folding of peptide results in a protein

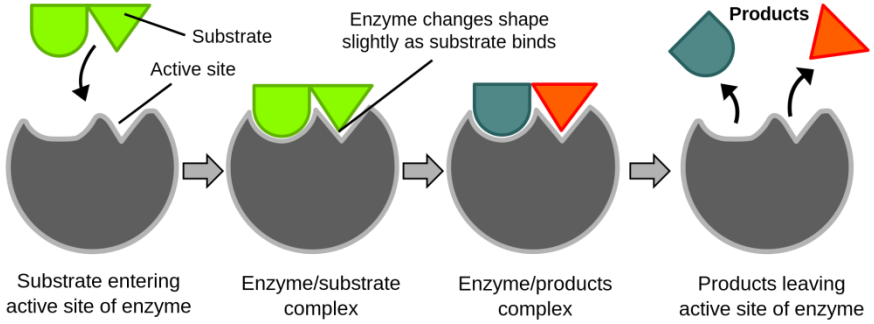
# What do proteins do?

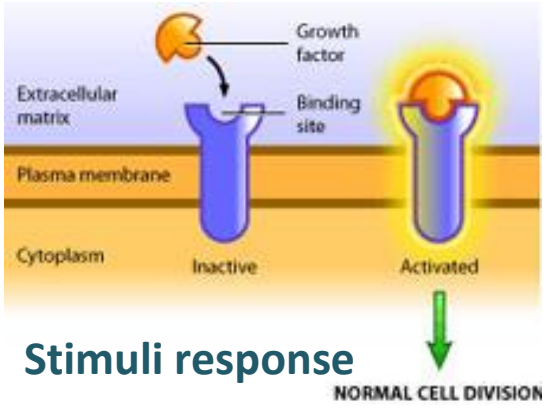
Proteins are essential to life and play a significant role in almost every biological function, including:




## Inter/intracellular transport

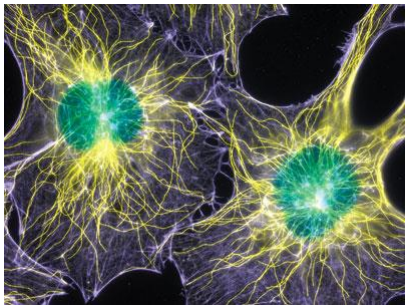
## Catalysing metabolic reactions

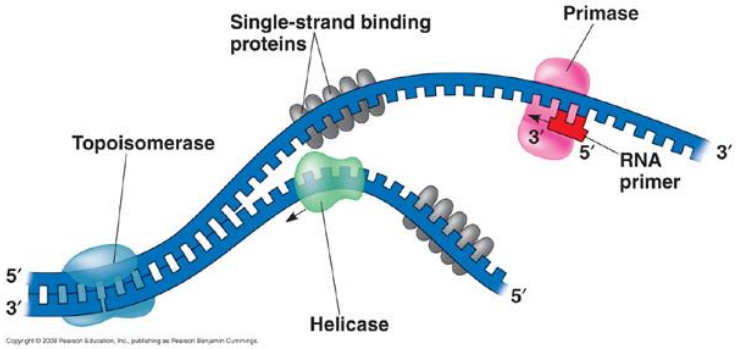



## Stimuli response

## Structural components

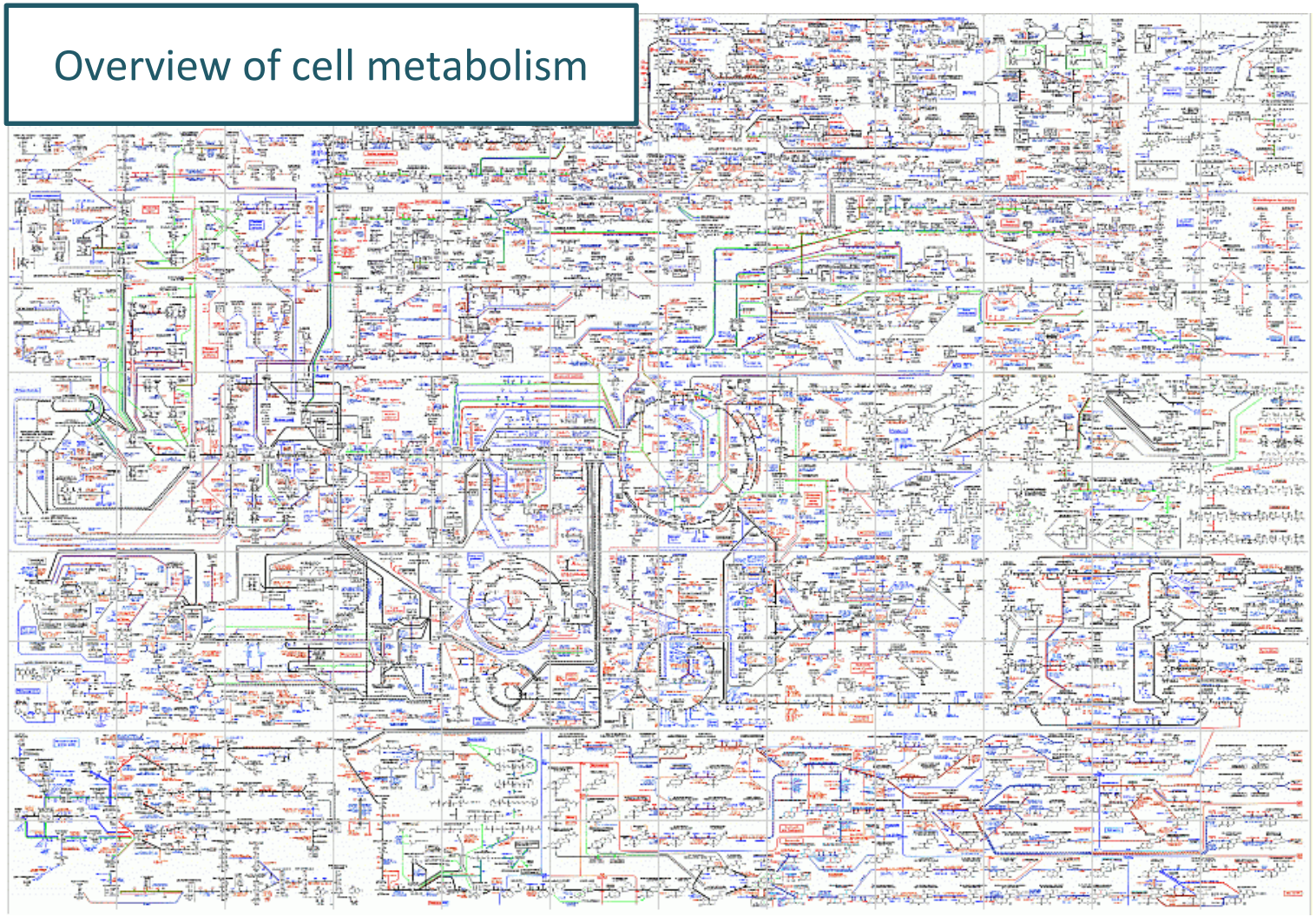





## DNA replication

# Controlled protein expression is essential

Overview of cell metabolism



# But it can go wrong

WE ARE MACMILLAN. CANCER SUPPORT

CANCER RESEARCH UK

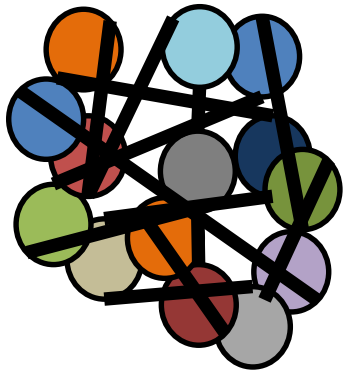
The Breast Cancer Research Foundation

TEENAGE CANCER TRUST

TOGETHER WE CAN STOP DIABETES
American Diabetes Association.

DIABETES UK
CARE. CONNECT. CAMPAIGN.

Abnormal protein regulation can lead to a wide variety of diseases



British Heart Foundation

HEART & STROKE FOUNDATION OF NEWFOUNDLAND & LABRADOR
Finding answers. For life.

# A real-life example

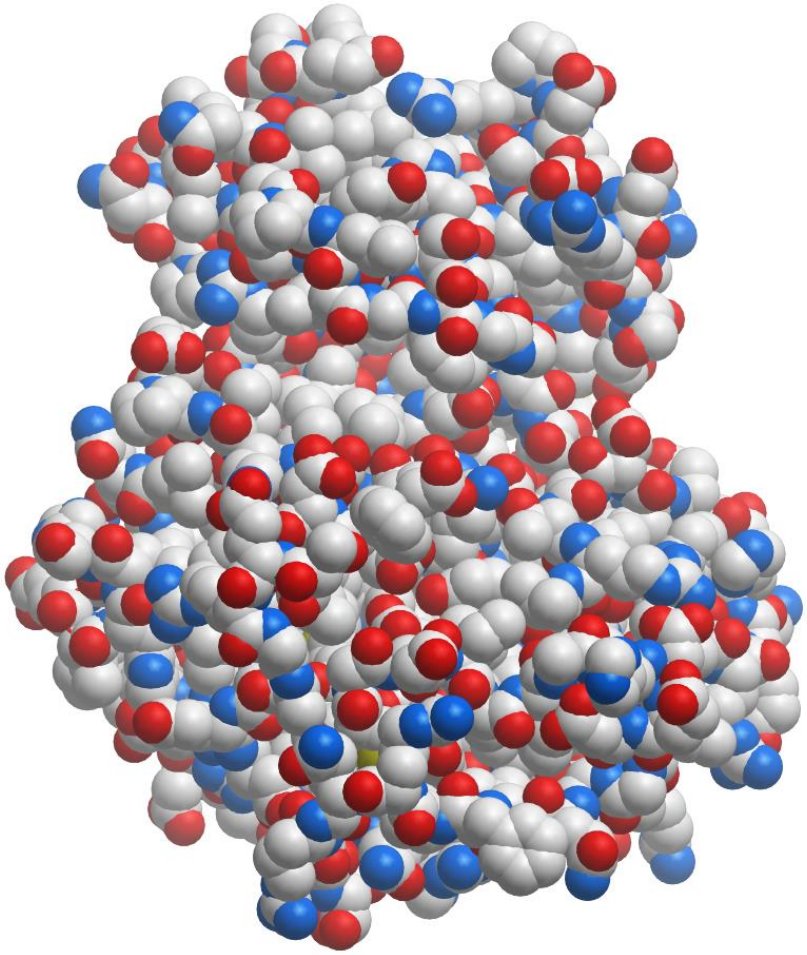
**Human PIM1**

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.



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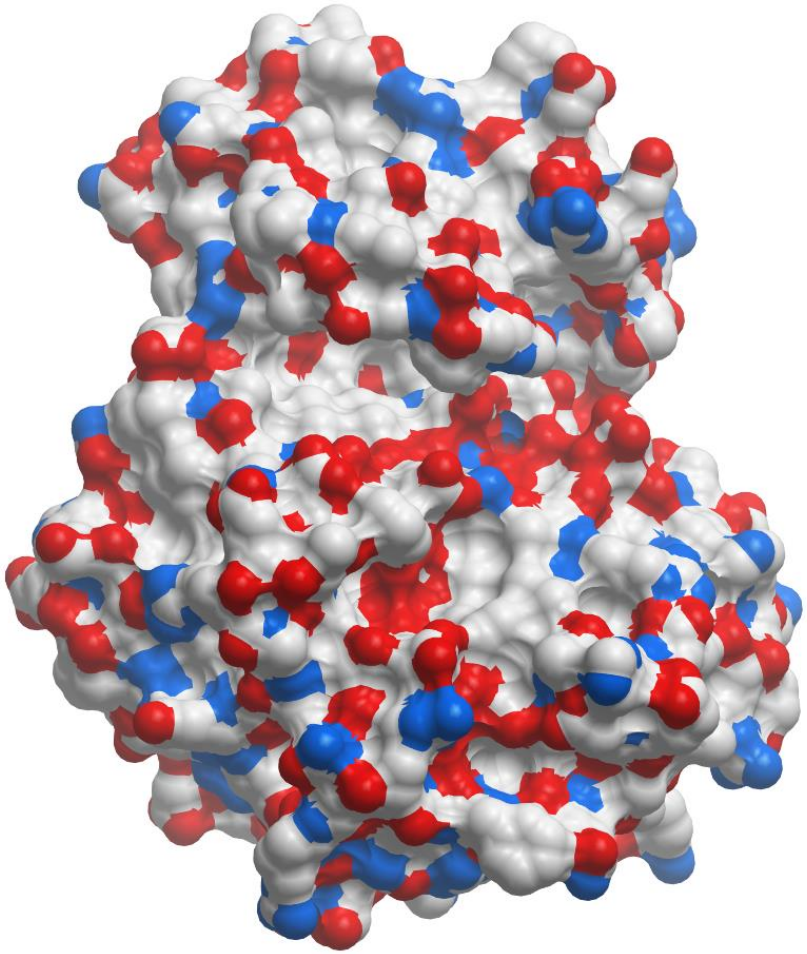

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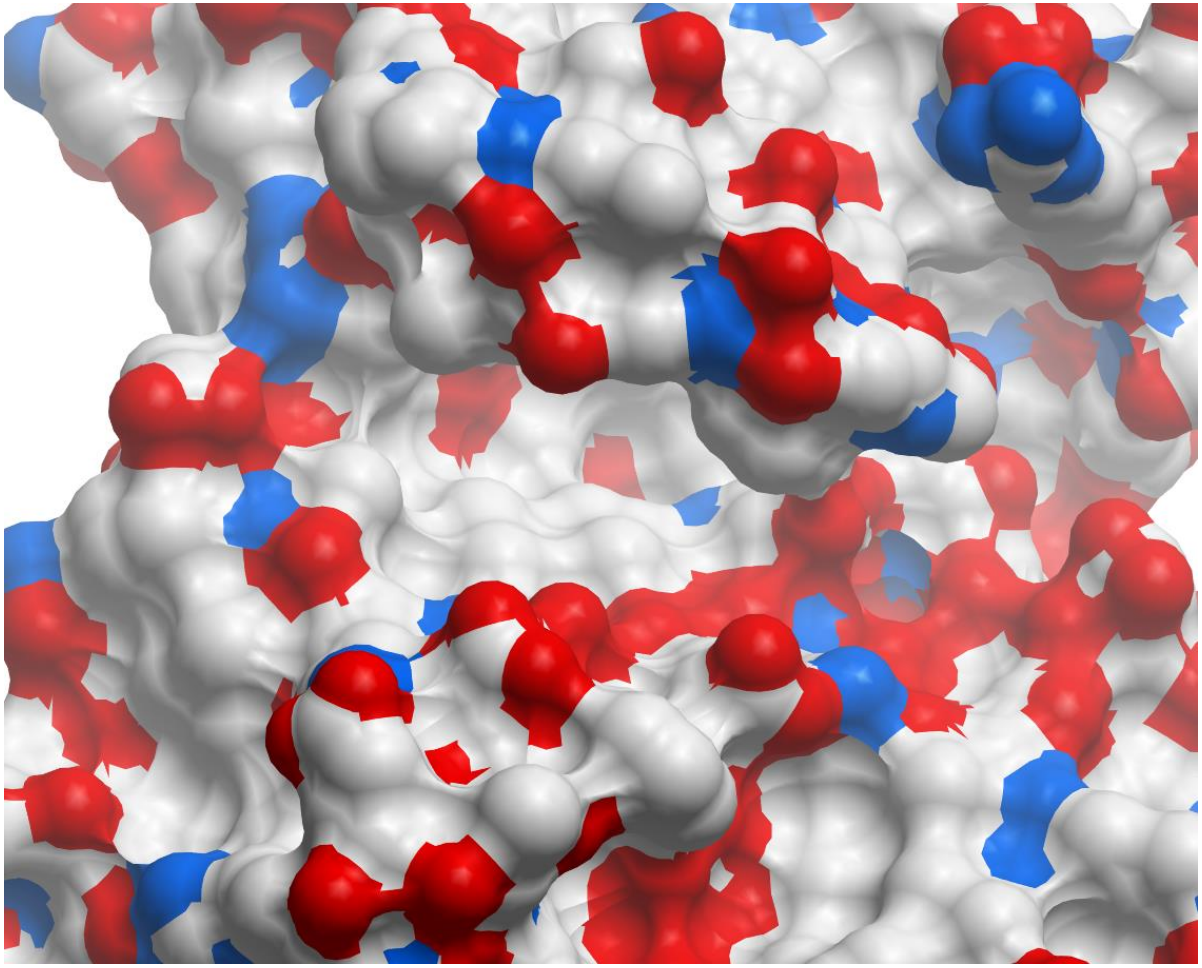

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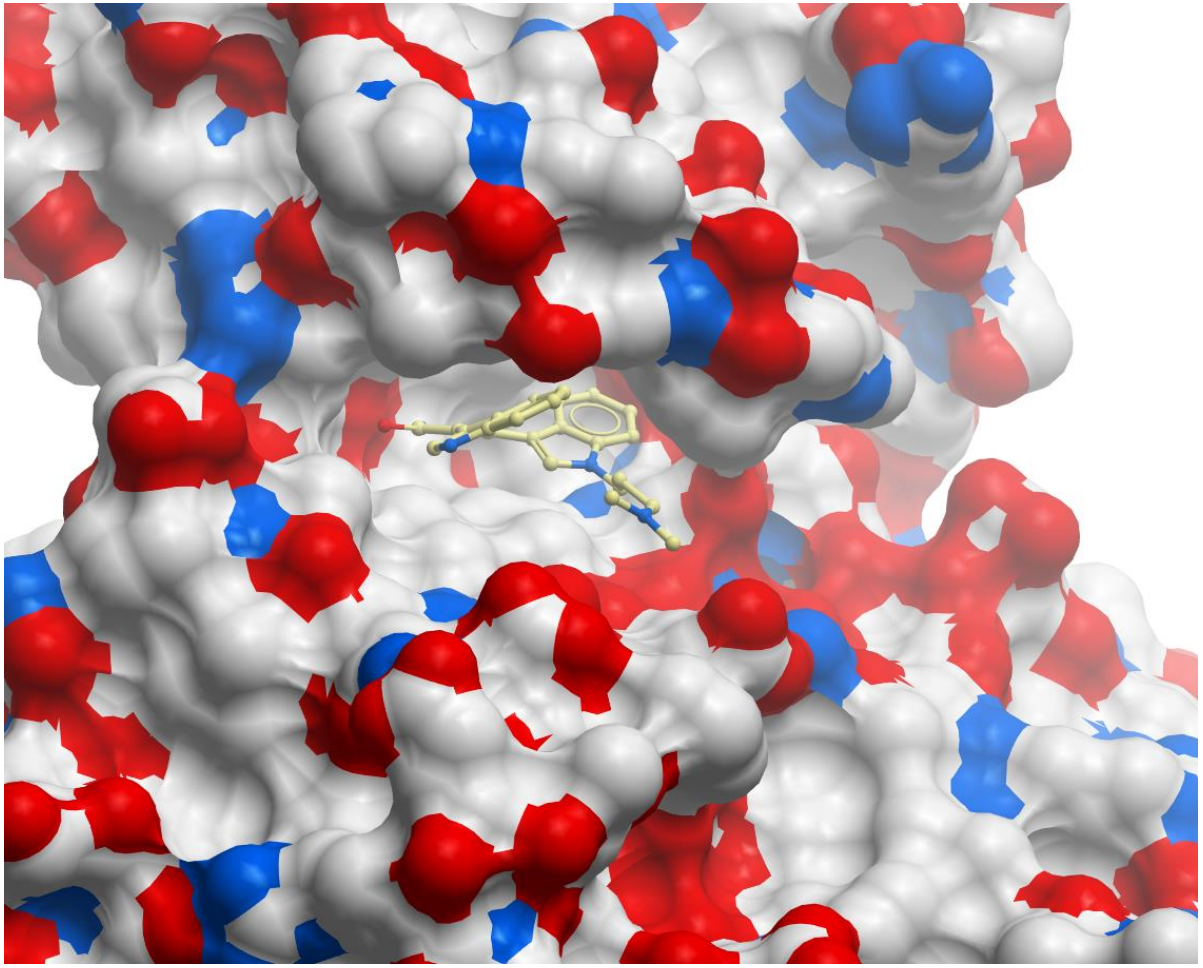

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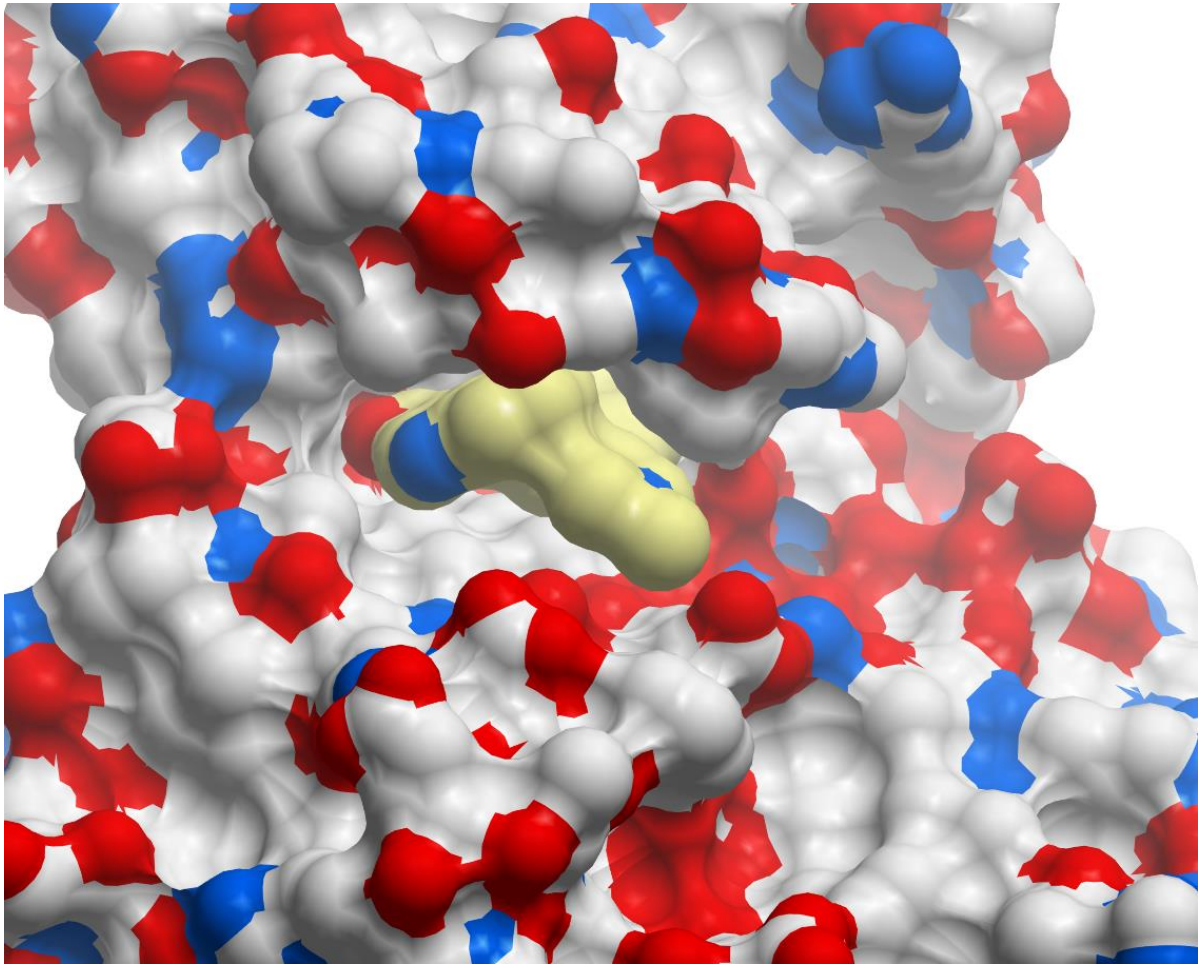

# What is an assay?

"an analytic procedure for qualitatively assessing or quantitatively measuring the presence, amount or functional activity of a target entity (the analyte)".

- Depending on the question, there are any number of potential assay types available
- Picking the most appropriate assay is crucial
- But knowing what is available and how to implement it is not easy

Kinetic assays
Bioassays
Ligand binding assays
Fluorescence assays
Colony count assays
Photometric assays
Absorbance assays
Immunoassays

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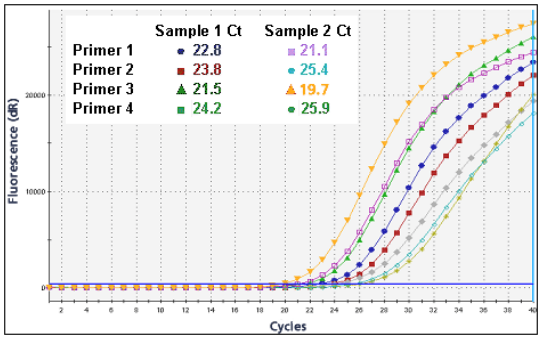
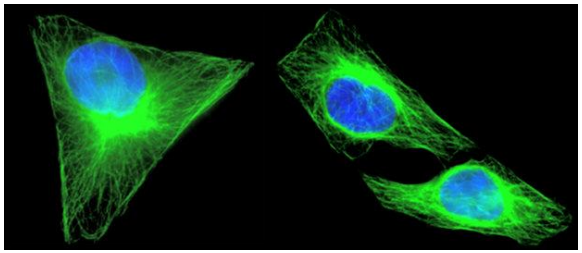
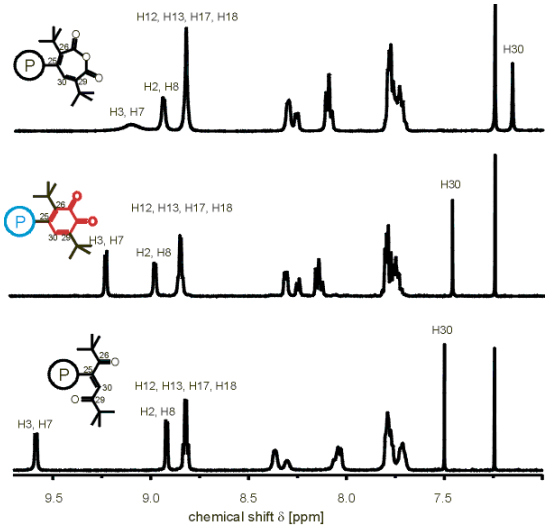
# Generic assay (meta) data capture is very challenging




qPCR data

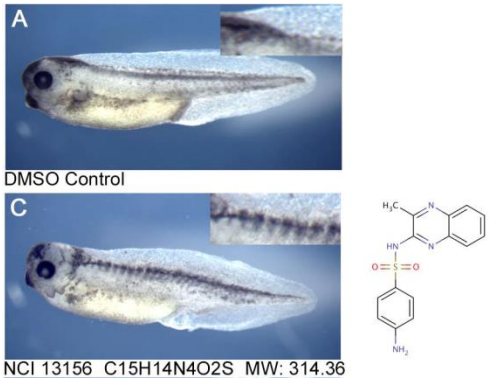


Immunostaining

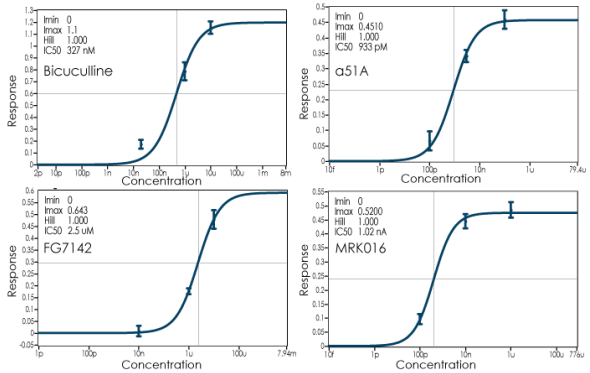



NMR spectra

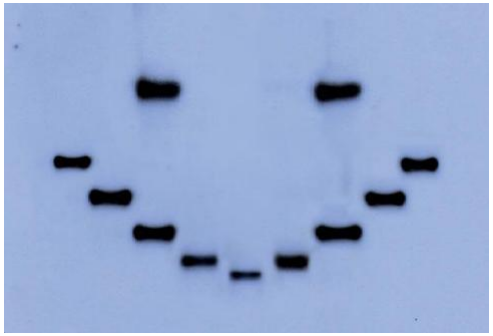
There is an incredibly diverse variety of assay data types




Phenotypic data




$IC_{50}$ data



Western Blot

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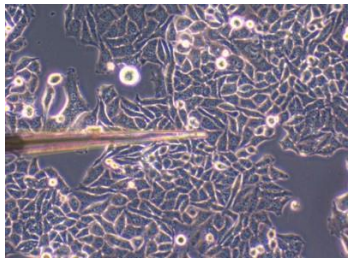
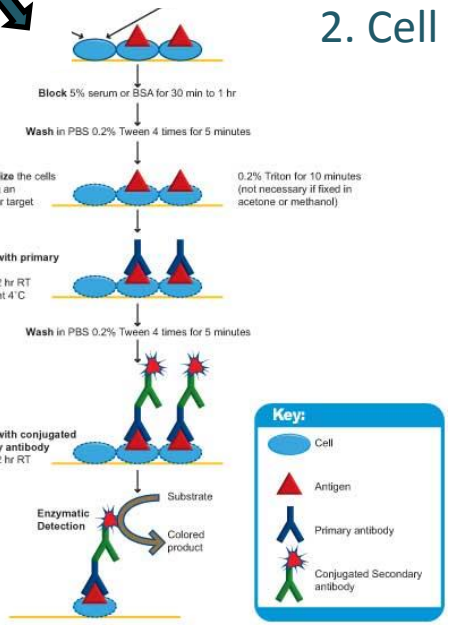
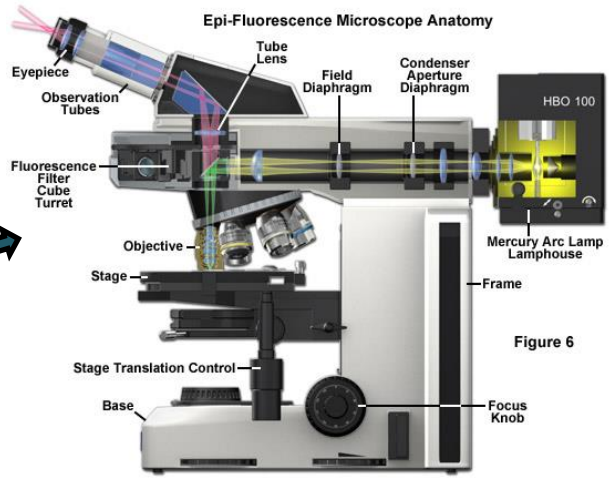
# Generic immunofluorescence protocol



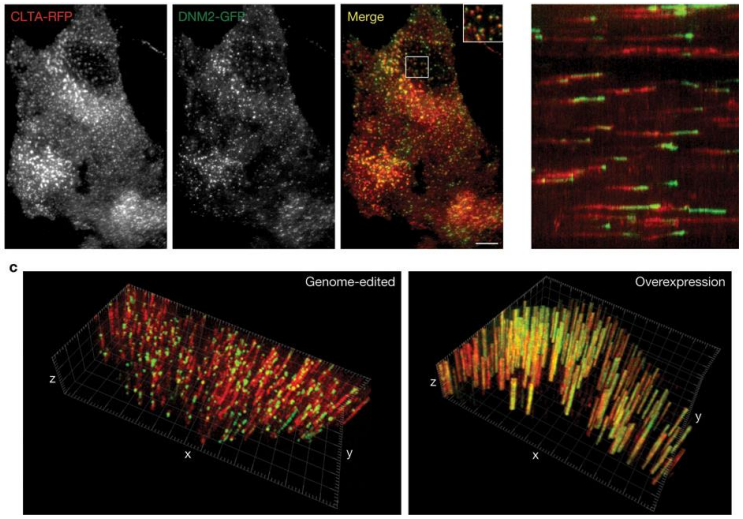
1. Cell culture




2. Cell staining




3. Fluorescence microscopy




4. Image analysis

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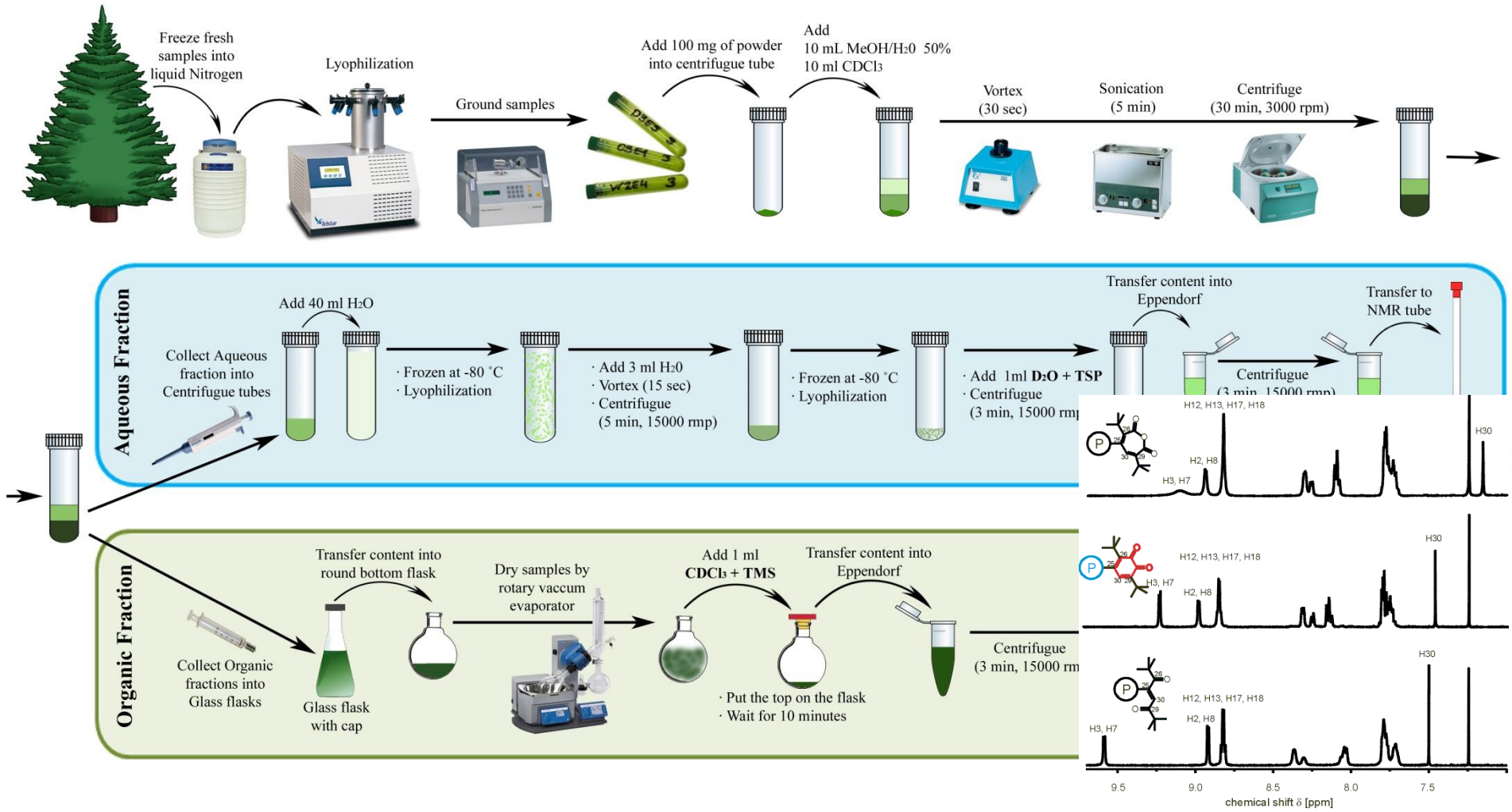
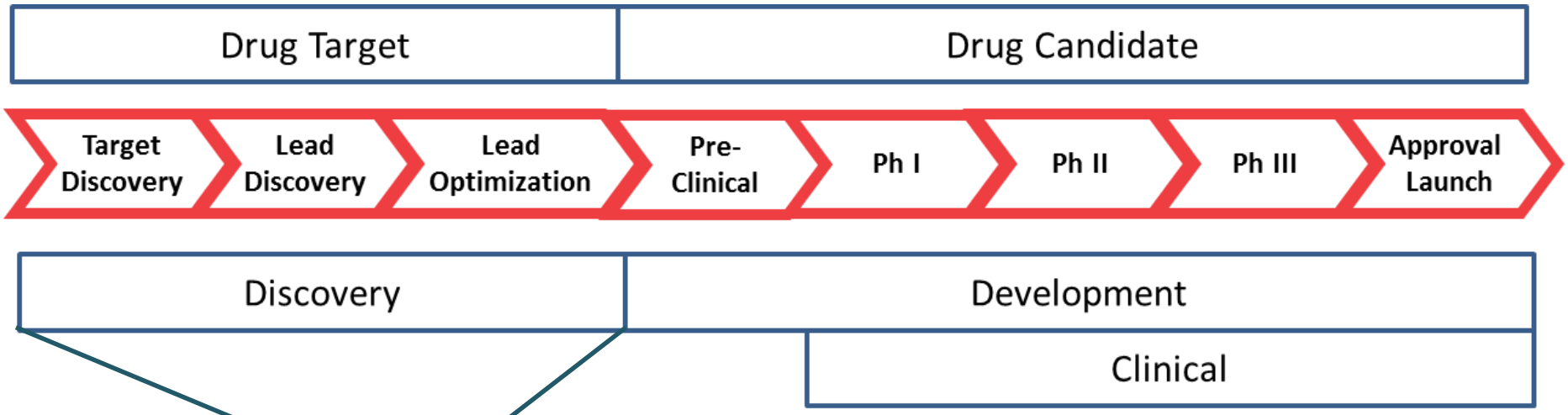
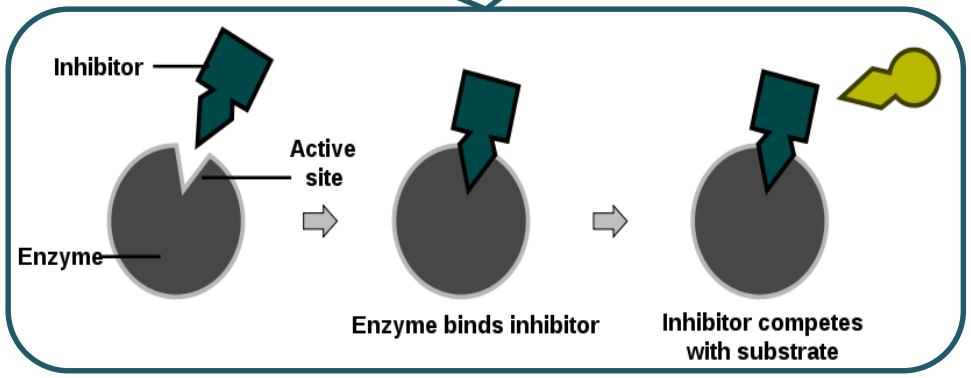
# Generic NMR protocol




WHAT'S SCIENCE EVER DONE FOR US?

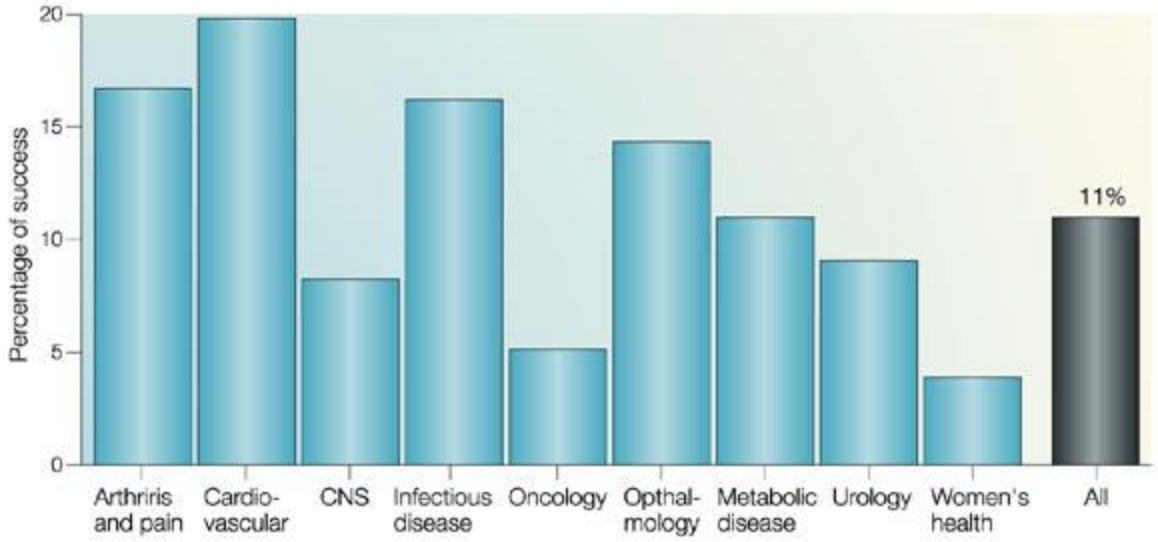
# Target focused small molecule drug discovery




Carefully selected small molecule inhibitors modulate a specific protein to induce a therapeutic effect.

# Drug discovery is hard




**Drug approval rates by therapeutic area**

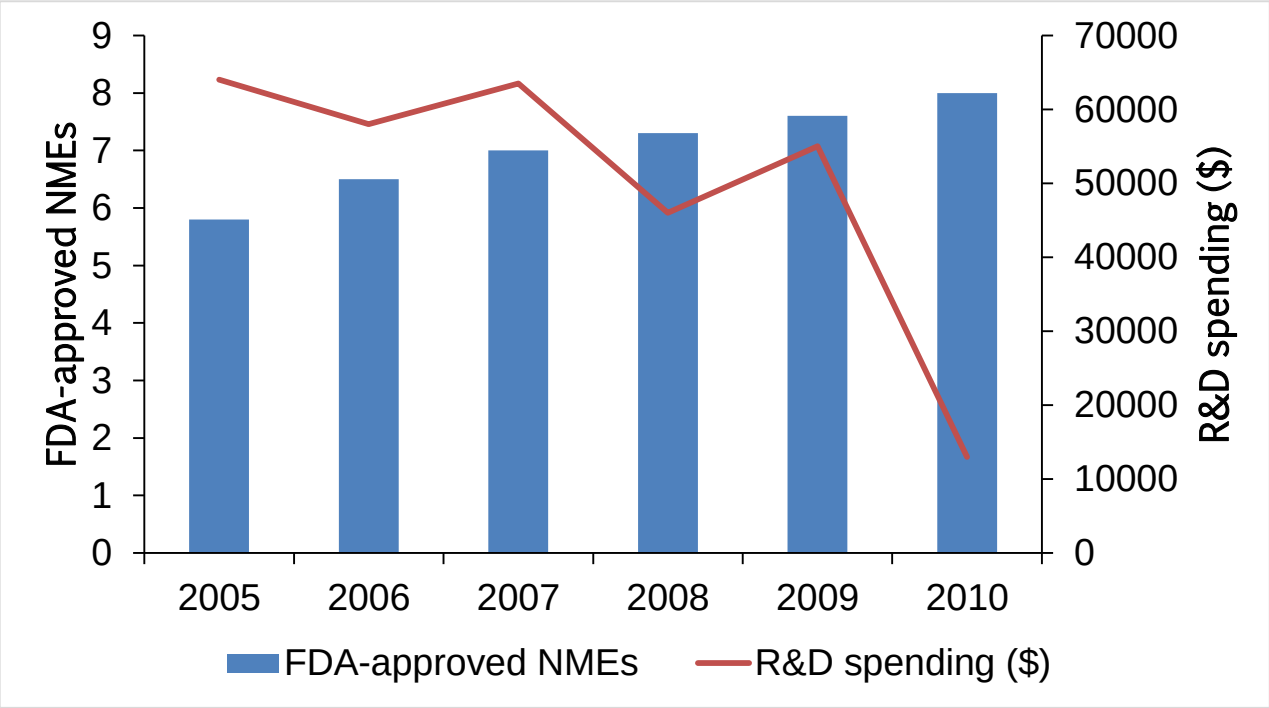
Many factors to consider when considering drug design –

- Chemical properties
- Adsorption, distribution, metabolism and excretion
- Pharmacokinetic profile
- Toxicity profile
- Off targets affects
- Target binding efficacy

http://hmg.oxfordjournals.org/content/early/2014/07/01/hmg.ddu309.full

# Attrition is high

## Summary of large pharma productivity between 2005-2010




Current attrition rates are unacceptably high
Time for a change in tactic

Taken from (Bunnage, 2011).

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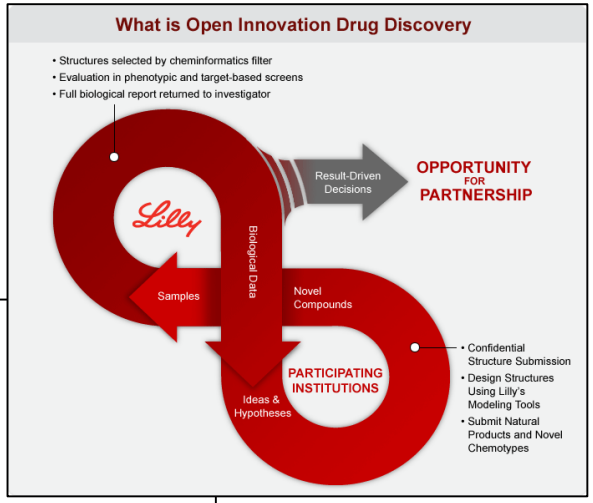
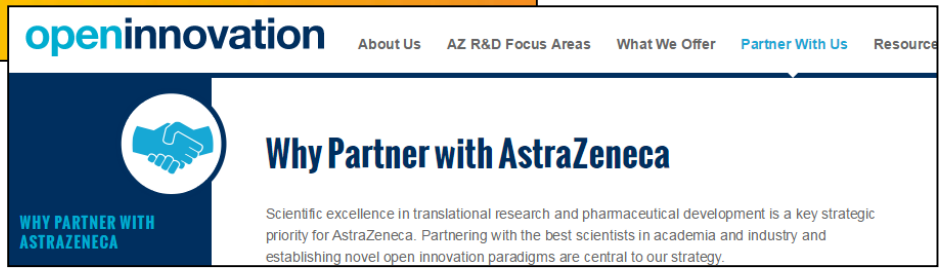
# Industry is moving to Open Innovation strategy

- Looking for new basic science in academia
- Why?
  - Access ‘blue-sky’ research
  - New assays, targets, starting points…
- Carrot?
  - Academic gets access to industry facilities and know-how




gsk GlaxoSmithKline Consumer Healthcare

**Maximising Open Innovation**



OK, fine.

But what's the problem in Oxford?

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# Challenges for University Researchers

- **Good science**

  i.e. data management

- **Efficiency**

  duplication of effort

- **Fulfilling Grant Conditions**

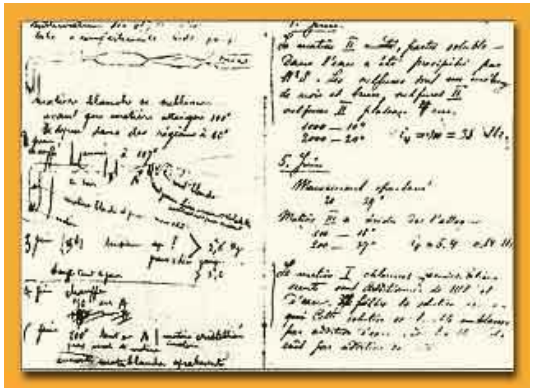
  open data

- **Personal progression**

  finding effective collaborators

- **Outcomes**

  partnerships with industry to bridge the gap



wellcome trust

NHS National Institute for Health Research

MRC Medical Research Council

# What sparked this all off?

"It is currently very difficult for one research group within the University to know if another group has expertise in a certain assay or screening technique. There is also no mechanism for one group to know if another group has compounds of interest for either target discovery or lead discovery."

**NDM/ISSF University-wide chemical biology audit - 2013**

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# Chemical biology across Oxford



Chemistry


WIMM


Pharm

NDORMS


Biochem


Oncology


Pathology

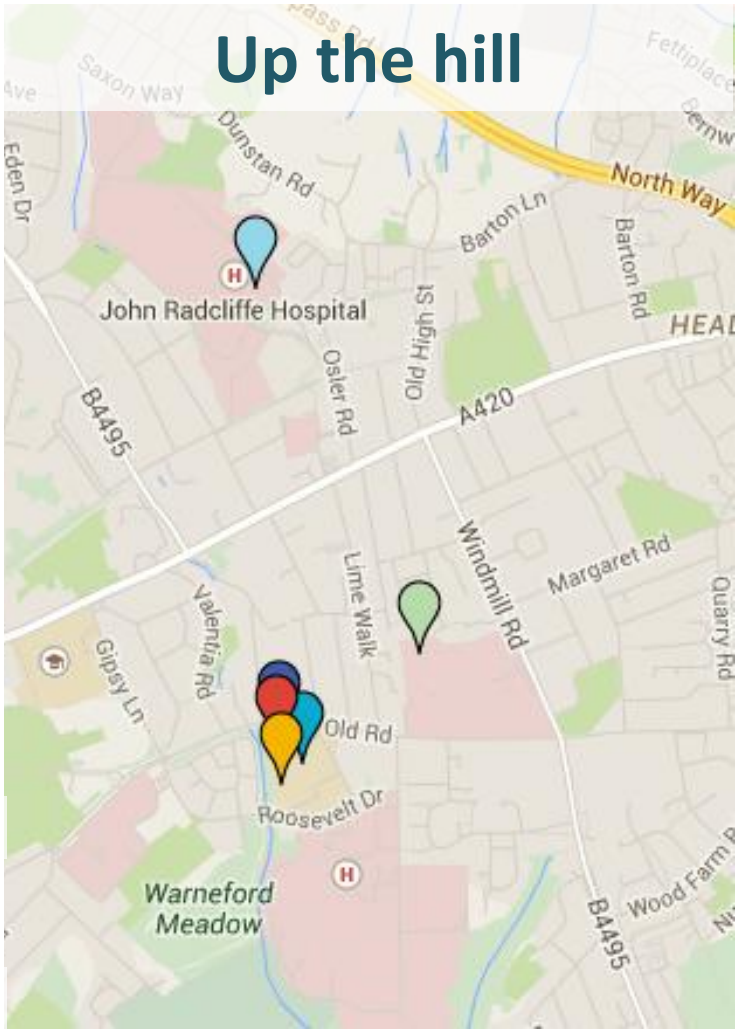

SGC


DPAG


TDI


STRUBI


WTCHG



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Bio Hub

# ChemBio … say

We approache… asked them about:

- What th… ing)
- What th…
- Whethe… rrently did

Lots don't use a… paper and pen a…

Sharing was not v… e benefit

Searching and bet… ies

# Hasn't this already been fixed?

## Sure, there are lots of tools available.

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ChemBio Hub

# We initiated what became known as ChemBio Hub

In response to the audit findings we secured funding from:


The ChemBio Hub vision:

- to provide the tools that will make it easier for Oxford University scientists to connect with colleagues to improve their research
- to satisfy funders that the data they have paid for is being managed according to their requirements
- to make new alliances with pharma and biotech partners.

# 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

# To provide:

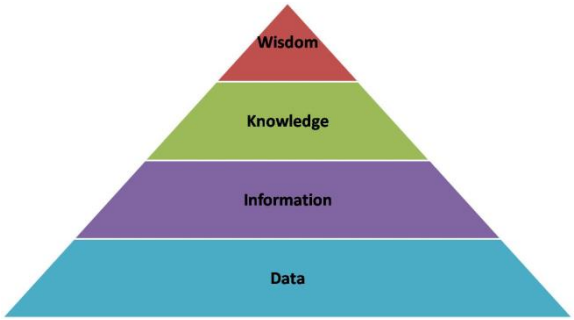
Better **reproducibility**

"..though the testimony of a single witness shall not suffice to prove the accused party guilty of murder; yet the testimony of two witnesses …shall ordinarily suffice to prove a man guilty"

More **discoverable**: easily find out *who* else has worked on similar compounds, what effort is going into similar *targets*, what similar *techniques* or *equipment* are in use.

Better **tools**: to visualise data and aid interpretation

- Saves time in interpretation
- Makes troubleshooting much easier
- Clarifies communication



# So, we brought together:

A project manager:

Web developers:

A Knowledge Exchange coordinator:

And a data scientist:

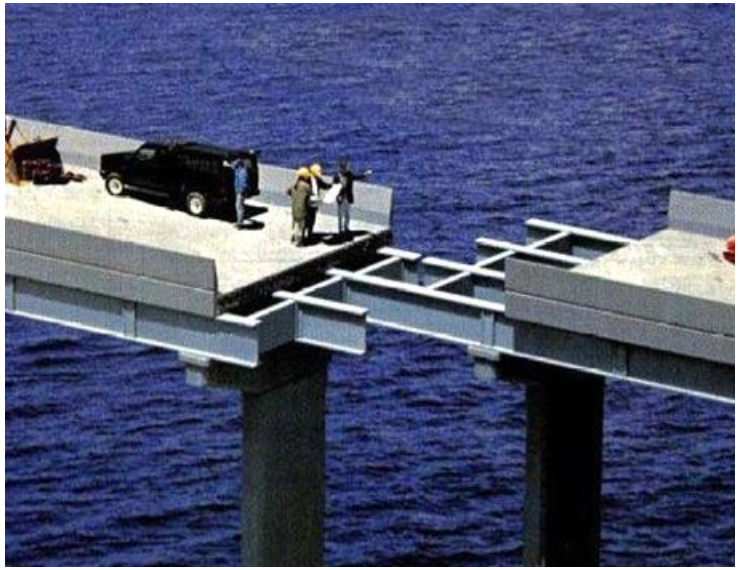
to tackle the problem.

The current funding will support the project until June 2016.

# How have we tackled it?


## One bite at a time

# Getting value to users



## Rather than risk this:

- Months of investigation and analysis
- Designing ‘the’ solution
- Unveiling to users – only to discover we’ve missed the mark

## We deliver functionality every 2 weeks:

- With a named individual in mind – fixing a specific problem
- Getting feedback straight away
- Without fear of negative findings – all results are of interest and influence further actions

Enough background.

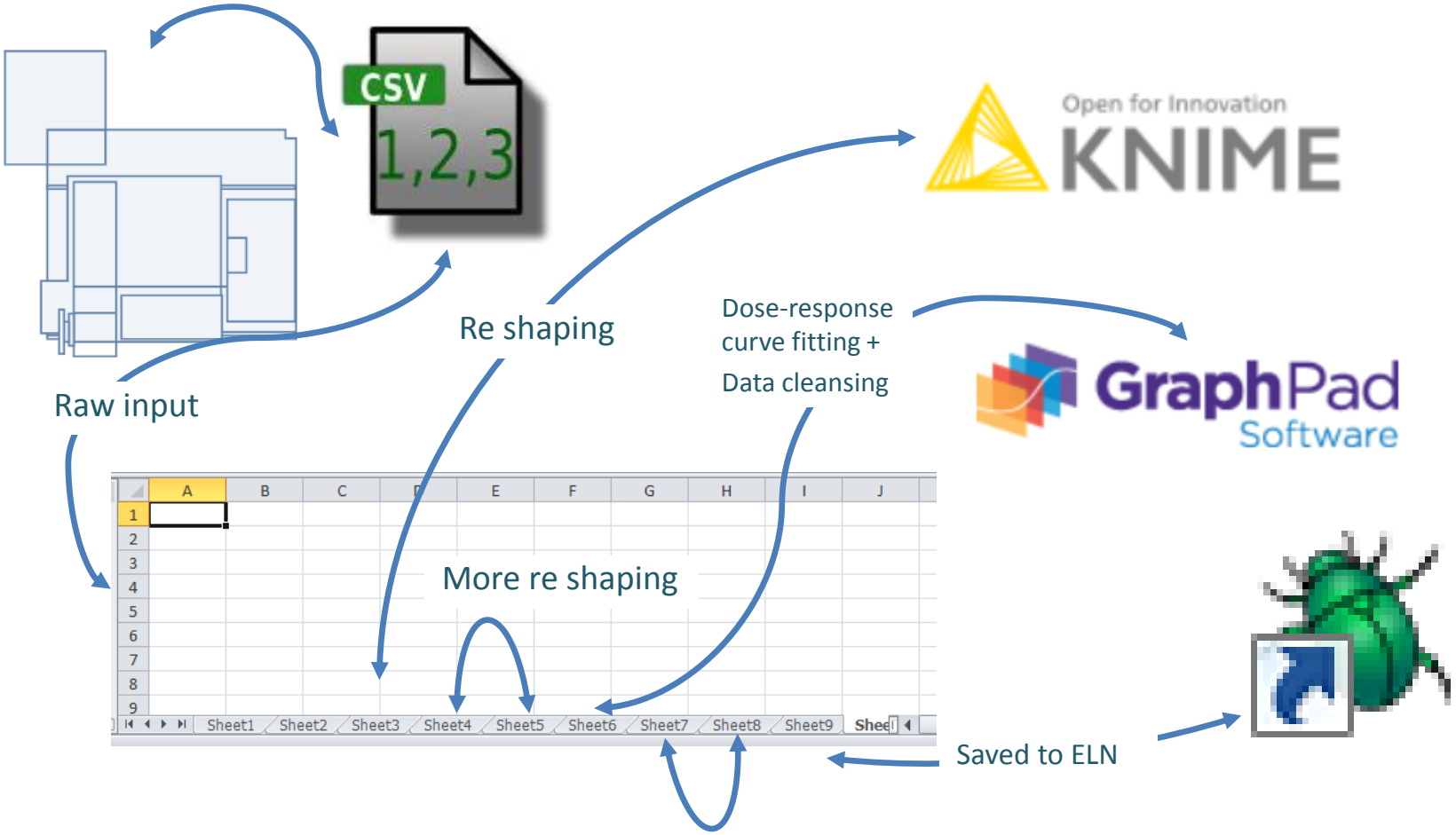
Show us some substance!

# Just a little bit more context

The first utility we built was ChemBio Crunch.

We took an existing workflow:

# Example Alpha Screen data flow from the TDI



# And we improved on it:

- Simplified the data flow
- Improved speed of processing
- Fixed quality issues along the way
- And made visualisation and sharing easier

# ChemBio Hub

## We came up with - ChemBio Crunch

### 1) Upload raw data

**Title***

**BMG output file***

Browse... No file selected.

**ESXX transfer file***

Browse... No file selected.

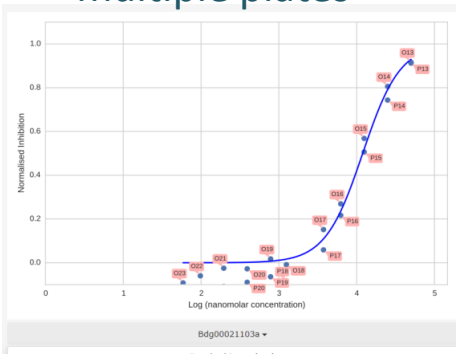
**Uploaded meta file**

Browse... No file selected.

Save

### 2) Validate plates for systematic errors

### 3) Calculate $IC_{50}$ for multiple plates




Mark as poor fit

### 4) Mark poor fits where observed

| | A | B | C | D | E | F | graph |
|---|---|---|---|---|---|---|---|
| 1 | plate | coupound | logIC50 | ic50 (nM) | system_comments | user | |
| 2 | 2 | BDG00021060a | 4.25927396 | 18166.6127 | Low total inhibition, values could be inaccurate | no | |
| 3 | 2 | BDG00021344a | 4.8345796 | 68324.9943 | Low total inhibition, values could be inaccurate | no | |
| 4 | 2 | BDG00019351a | 4.41049146 | 25733.0618 | Low total inhibition, values could be inaccurate | no | |

Next Plate ❯ Export ▾

Export all workflow graphs as XLSX

### 5) Export and deposit in ELN (Comments automatically generated where $IC_{50}$ may be inaccurate)

# Results

- Production-ready web application written in 3 weeks
- ChemBio Crunch matches the GraphPad curve fit to within <1% error
- Time to process plates cut by > 10x

"I was just looking at the concentration discrepancies you mentioned and it looks to me like there has been copy and paste error or the template is out of date... If this is the case then it is the kind of thing that would be eliminated by using the new utility!"

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ChemBio Hub

# ChemBio Hub Crunch

ChemBio Crunch - The assay data analyser

Paul | Log Out

Prev Plate

## Plate [3]-01 (3 of 3 total plates imported)

Next Plate | Export

- Your data is displayed as a conditionally formatted heatmap
- Validate your data by eye.
- You can deselect wells as outliers by clicking the value in each table cell. Deselected cells will turn grey.
- You can deselect columns and rows by clicking on the label.
- You can re-select cells by clicking the value again.
- When you are finished, click Update and you will see the graphs below

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| A | 940k | 927k | 911k | 921k | 896k | 907k | 894k | 907k | 876k | 893k | 909k | 905k | 898k | 901k | 885k | 873k | 882k | 882k | 891k | 901k | 915k | 920k | 919k | 924k |
| B | 863k | 827k | 829k | 814k | 829k | 815k | 801k | 805k | 801k | 820k | 803k | 801k | 795k | 819k | 823k | 815k | 809k | 801k | 850k | 846k | 847k | 846k | 851k | 908k |
| C | 635k | 699k | 761k | 784k | 793k | 818k | 800k | 810k | 772k | 777k | 794k | 770k | 422k | 401k | 511k | 601k | 674k | 748k | 752k | 745k | 779k | 794k | 794k | 825k |
| D | 633k | 665k | 723k | 756k | 752k | 741k | 759k | 745k | 772k | 759k | 749k | 767k | 378k | 413k | 500k | 583k | 665k | 726k | 743k | 777k | 773k | 801k | 797k | 857k |
| E | 319k | 694k | 776k | 791k | 773k | 779k | 755k | 753k | 745k | 746k | 754k | 748k | 2565 | 2356 | 27k | 260k | 560k | 685k | 738k | 717k | 741k | 766k | 772k | 785k |
| F | 310k | 670k | 758k | 743k | 738k | 741k | 727k | 730k | 729k | 742k | 745k | 724k | 1425 | 1938 | 27k | 257k | 582k | 697k | 744k | 745k | 739k | 753k | 788k | 842k |
| G | 3705 | 46k | 357k | 628k | 725k | 706k | 724k | 716k | 756k | 737k | 747k | 744k | 3116 | 1045 | 1710 | 3990 | 65k | 405k | 618k | 697k | 703k | 771k | 745k | 794k |
| H | 3287 | 46k | 348k | 601k | 672k | 696k | 720k | 711k | 713k | 722k | 718k | 724k | 1520 | 1083 | 1387 | 4009 | 64k | 418k | 636k | 712k | 727k | 749k | 780k | 824k |
| I | 738k | 725k | 719k | 726k | 704k | 720k | 701k | 739k | 714k | 710k | 729k | 721k | 2869 | 1634 | 2964 | 48k | 311k | 605k | 666k | 695k | 702k | 698k | 722k | 757k |
| J | 716k | 693k | 695k | 689k | 726k | 688k | 683k | 737k | 688k | 708k | 705k | 704k | 1938 | 1634 | 2622 | 47k | 317k | 606k | 661k | 693k | 712k | 724k | 735k | 789k |
| K | 801k | 771k | 755k | 744k | 733k | 733k | 727k | 744k | 724k | 737k | 739k | 720k | 760k | 749k | 726k | 732k | 748k | 742k | 764k | 739k | 766k | 751k | 771k | 797k |
| L | 758k | 726k | 731k | 726k | 721k | 746k | 717k | 723k | 722k | 721k | 709k | 736k | 736k | 737k | 734k | 738k | 746k | 743k | 755k | 743k | 750k | 759k | 801k | 846k |
| M | 806k | 772k | 747k | 751k | 743k | 748k | 752k | 736k | 742k | 740k | 742k | 726k | 747k | 744k | 751k | 745k | 748k | 752k | 761k | 751k | 741k | 758k | 780k | 821k |
| N | 798k | 749k | 750k | 728k | 729k | 724k | 730k | 737k | 735k | 730k | 726k | 735k | 740k | 734k | 738k | 745k | 763k | 742k | 749k | 771k | 786k | 779k | 805k | 855k |
| O | 100k | 432k | 637k | 689k | 720k | 729k | 724k | 726k | 728k | 732k | 713k | 722k | 728k | 736k | 724k | 736k | 740k | 744k | 753k | 744k | 733k | 759k | 783k | 815k |
| P | 84k | 425k | 675k | 727k | 754k | 758k | 767k | 785k | 763k | 783k | 769k | 787k | 785k | 771k | 782k | 776k | 782k | 773k | 791k | 791k | 790k | 841k | 852k | 920k |

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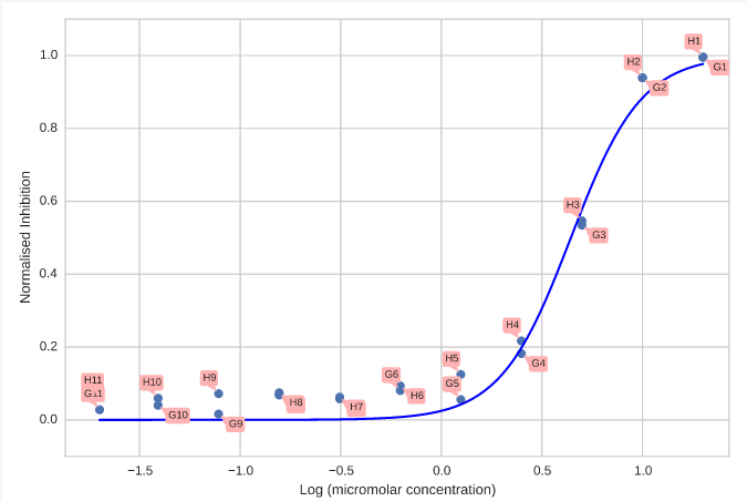
ChemBio Hub

# ChemBio Hub Crunch

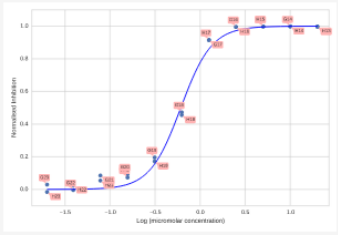
| | | | | | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| N | 798k | 749k | 750k | 728k | 729k | 724k | 730k | 737k | 735k | 730k | 726k | 735k | 740k | 734k | 738k | 745k | 763k | 742k | 749k | 771k | 786k | 779k | 805k | 855k |
| O | 100k | 432k | 637k | 689k | 720k | 729k | 724k | 726k | 728k | 732k | 713k | 722k | 728k | 736k | 724k | 736k | 740k | 744k | 753k | 744k | 733k | 759k | 783k | 815k |
| P | 84k | 425k | 675k | 727k | 754k | 758k | 767k | 785k | 763k | 783k | 769k | 787k | 785k | 771k | 782k | 776k | 782k | 773k | 791k | 791k | 790k | 841k | 852k | 920k |

**Bdjjb009570a**



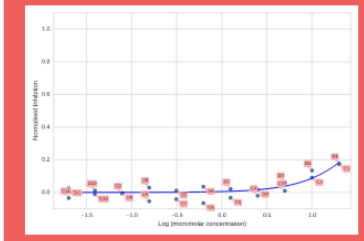

Good Curve

**Bdv00005348a**



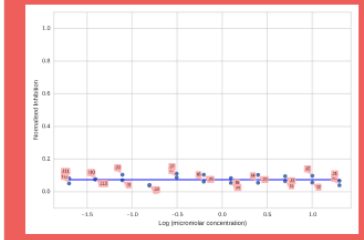
Good Curve

**Bdjjb008930b**



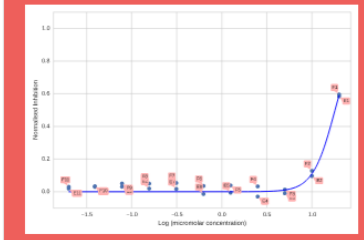
inactive compound

**Bdjjb009571a**



inactive compound

**Bdjjb008841k**



Top plateaus at below 80%

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# The technology stack

## What you see





## What that runs on








## What we use to deploy and test it

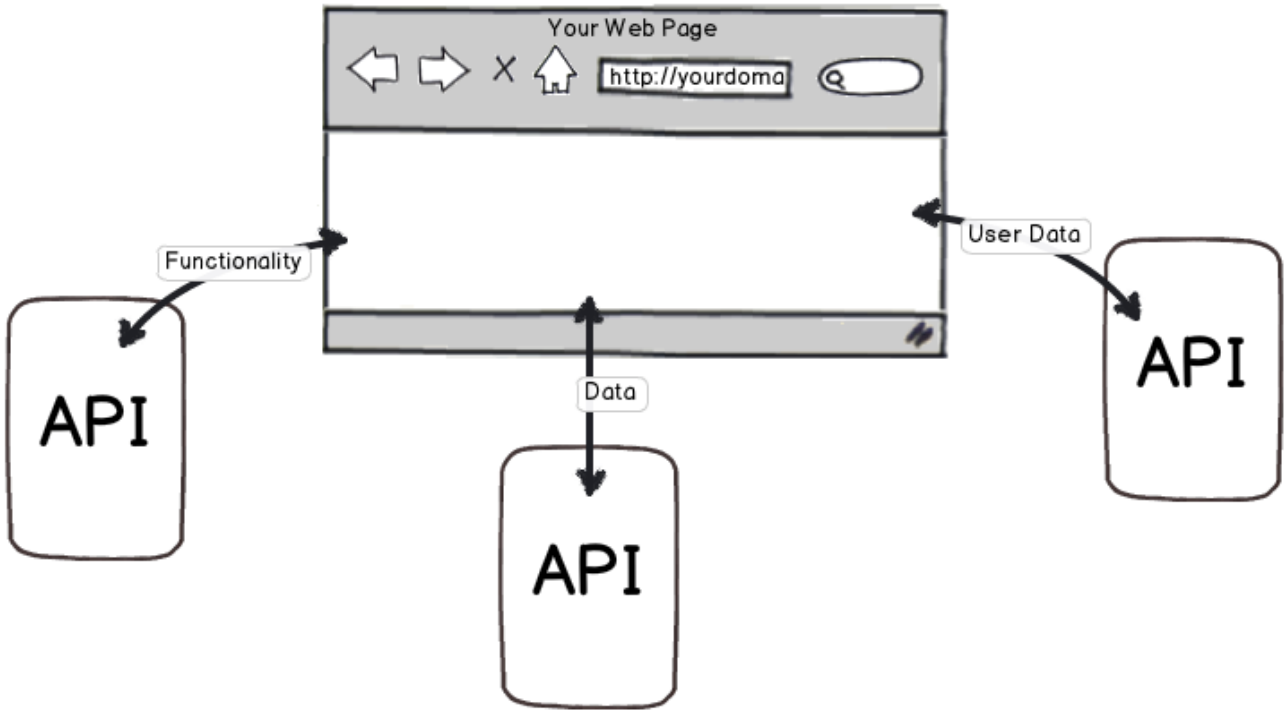






# Modular design for resilience and data sharing

- System should “talk” to other installations
- Modules should be self-contained



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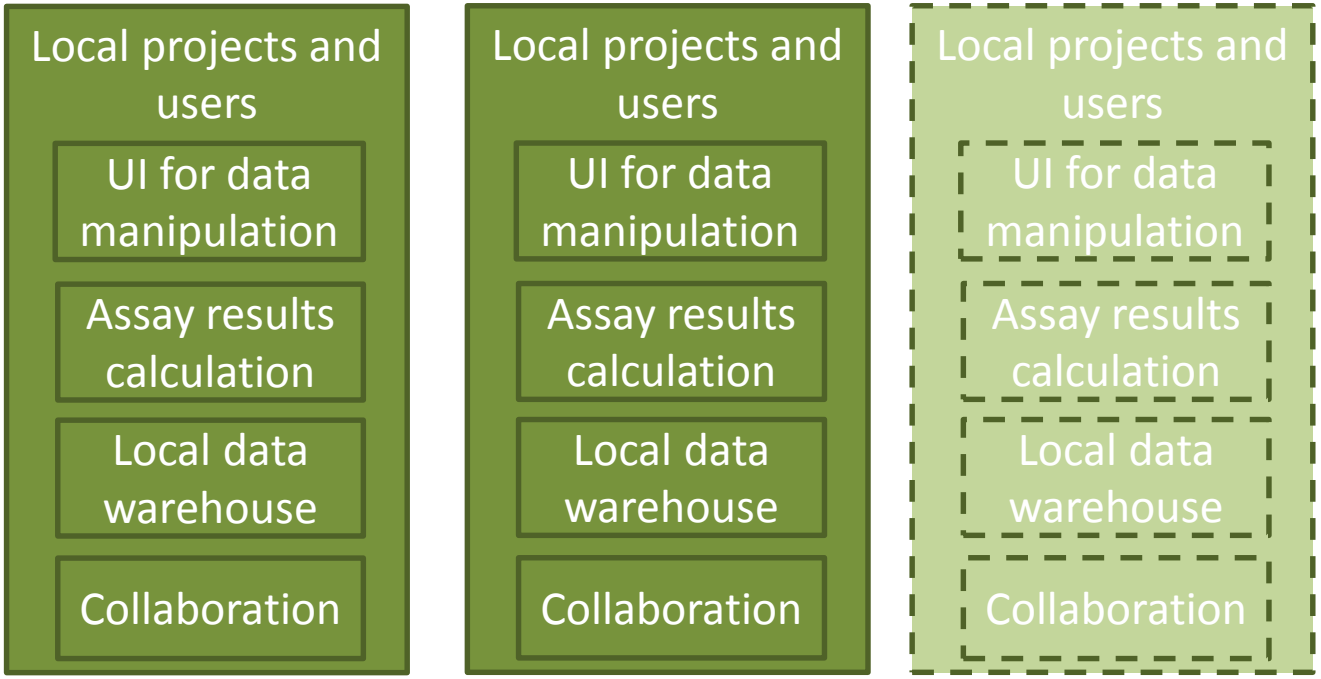
# High level architecture

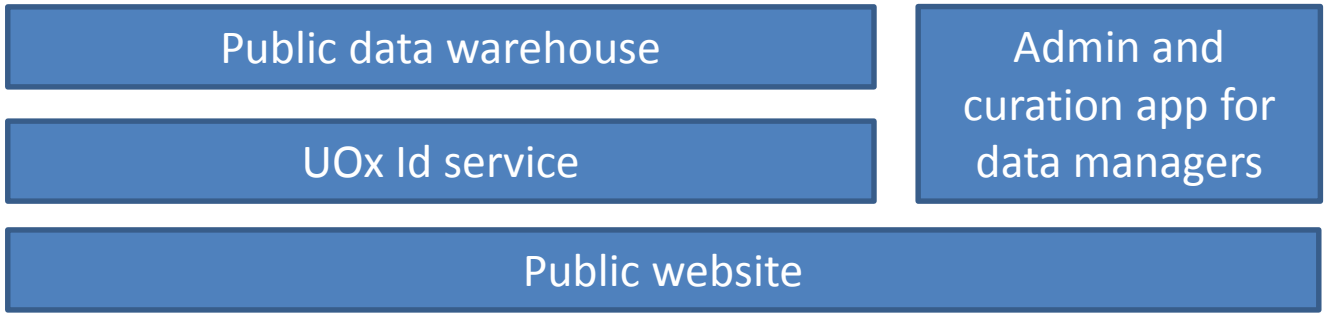
Silos for groups who want to collaborate together

Instance level services




Global services that all can connect to

Global Services



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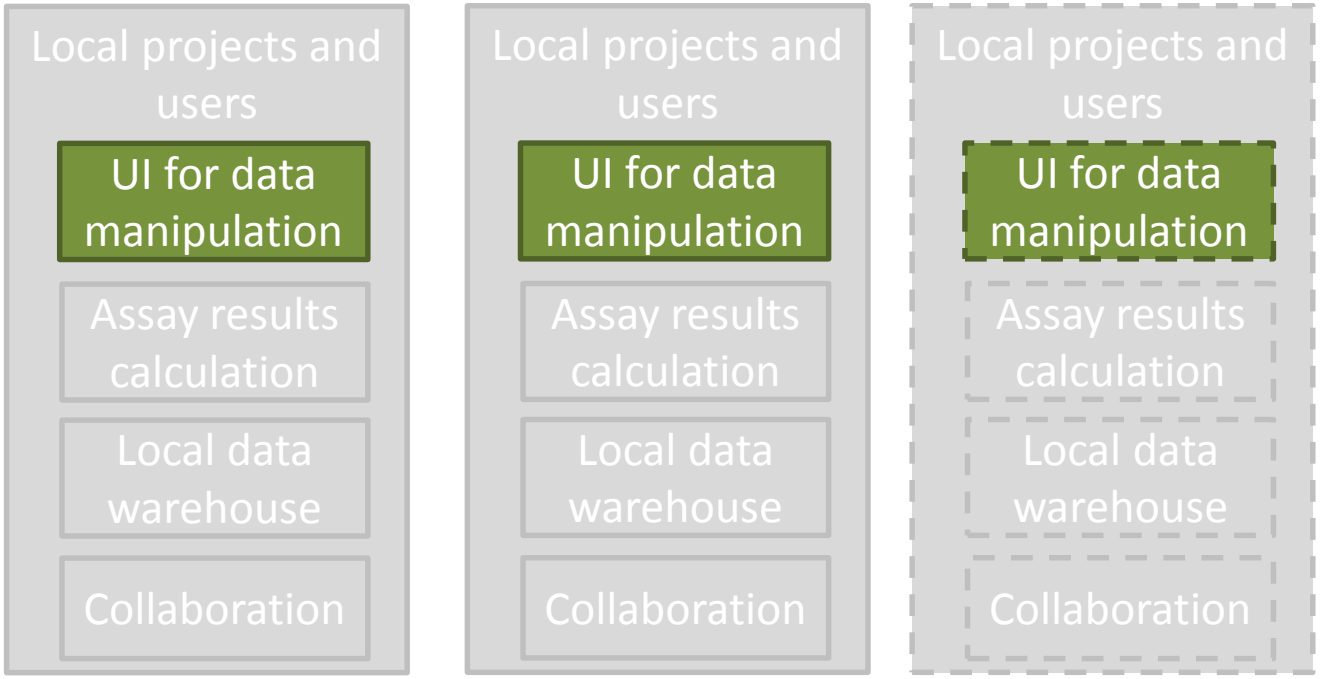
# Focus on Web Front End Technology

Silos for groups who want to collaborate together

Instance level services




Global services that all can connect to

Global Services

# Websites vs apps = different front end

- Jekyll static site for website and blog
  - Easy deployment
  - SEO friendly
  - No database or security issues
  - Easy deployment



[chembiohub.ox.ac.uk](chembiohub.ox.ac.uk)

ANGULARJS by Google

- AngularJS for apps
  - Easy-to-follow coding standards for javascript
  - Slick and customisable user experience without code repetition
  - Works with our API which we must develop anyway

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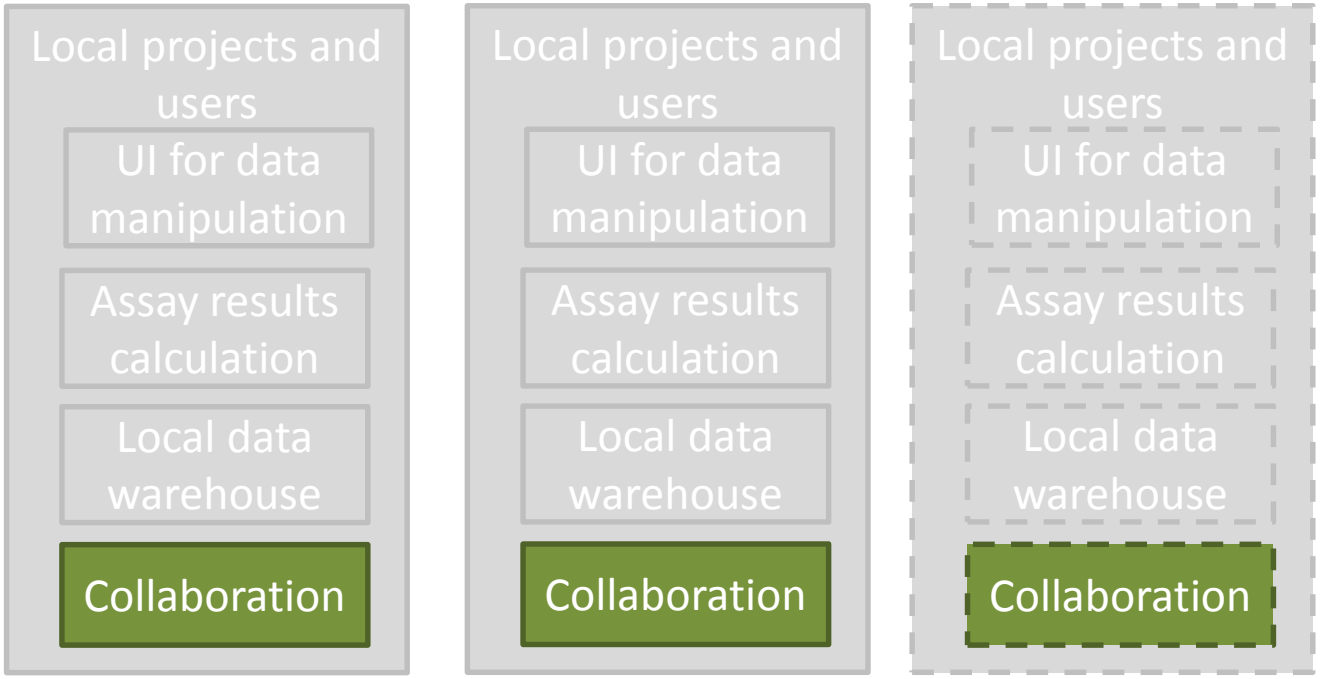
# Focus on Collaboration

Silos for groups who want to collaborate together

Instance level services




Global services that all can connect to

Global Services

# Existing tool for user feedback and Q and A

- Many tools purport to help people collaborate
  - Success can depend on the people and the situation more than the tool
- We chose a simple team messaging tool

  slack.com

- Integrated feedback button
- Slack users will be able to message the team and ask each other questions

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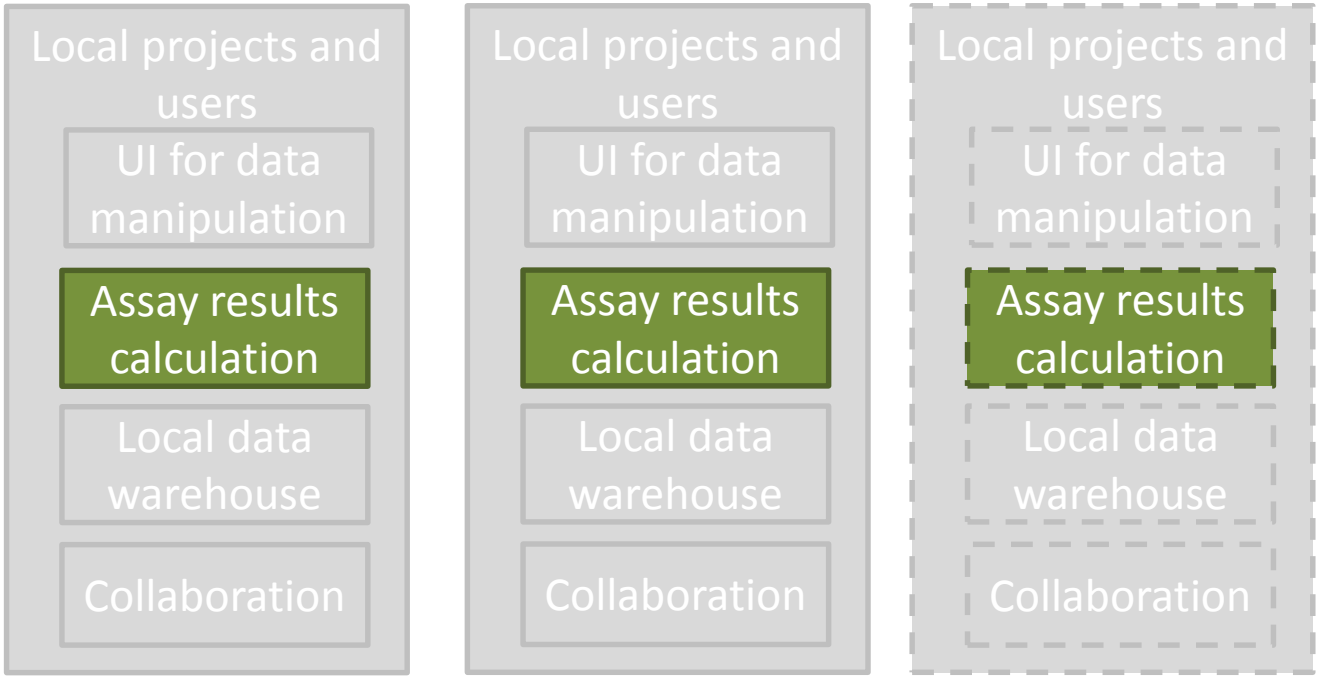
# Focus on Calculations and Data Editing

Silos for groups who want to collaborate together

Instance level services

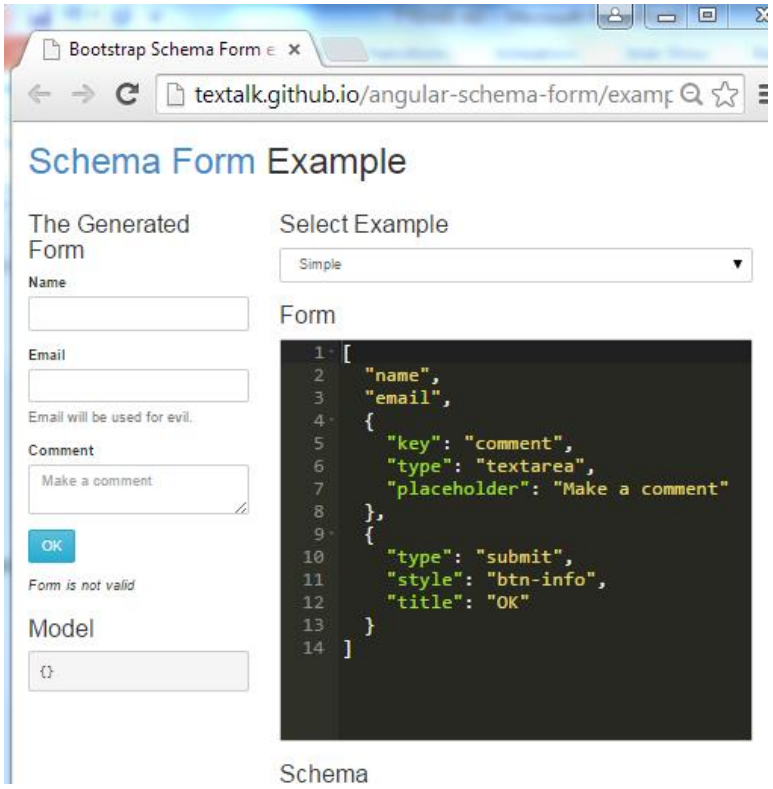



Global services that all can connect to

Global Services

# ChemBio Crunch and future curation apps

- Work with raw data and custom fields
  - Build forms in browser with angularjs and JSON Schema
- Open source calculation software
  - Python Pandas to import
  - Python LMFit for curve fitting
  - Matplotlib for graphing
  - RDKit and Openbabel for chemistry calculations



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# Focus on Data Storage and Transfer Formats

Silos for groups who want to collaborate together

Instance level services

Local projects and users

UI for data manipulation

Assay results calculation

Local data warehouse

Collaboration

Local projects and users

UI for data manipulation

Assay results calculation

Local data warehouse

Collaboration

Local projects and users

UI for data manipulation

Assay results calculation

Local data warehouse

Collaboration

Global services that all can connect to

Global Services

Public data warehouse

UOx Id service

Admin and curation app for data managers

Public website

# Backend Development and Databases

- PostgreSQL + HStore + RDKit extensions
  - Custom fields allowed
  - No custom nested objects
    - Too difficult to curate
- ChEMBL DB access code
  - Allows us to build the API we need
  - Avoids creating a new schema
  - Uses our preferred framework Django



# Data Transfer and Deposition

- ChemBio Hub will allow users to deposit their data in external services


- Where deposition APIs do not exist e.g. ChEMBL– we help build them
- Long term archiving in https://databank.ora.ox.ac.uk/
  - Single records will be packaged with files + json schema.
  - Private projects will be embargoed

# ChemBio Hub - Open Source is key

We are open source on Github

github.com/thesgc

GitHub

Important for reproducible, open science

Important for open collaboration

Important for open publications

Important for distributed deployment model

(virtual machines, less config to get software working)

Great!

What else have you done?

# ChemBio Hub ChemReg

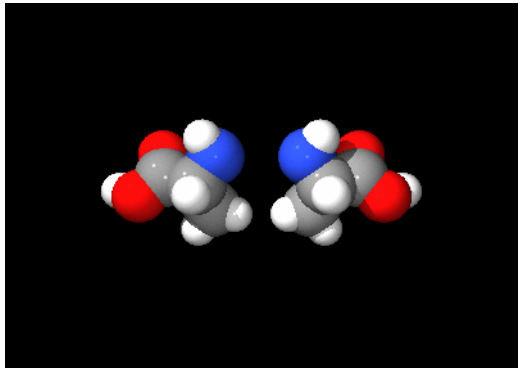
Compounds to be registered need to be uniquely identified. Users were concerned about sequential assignment inadvertently allowing others to deduce who had registered private compounds.

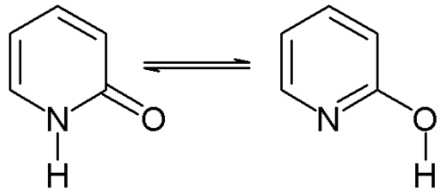
So we generate UOxIDs, in a number plate format:


Randomly generated, then checked to ensure they are unique.

The format UOX*aa*nn*bbb* will allow over 1bn combinations of relatively simple to remember identifiers

# ChemBio Hub ChemReg – registration complexity

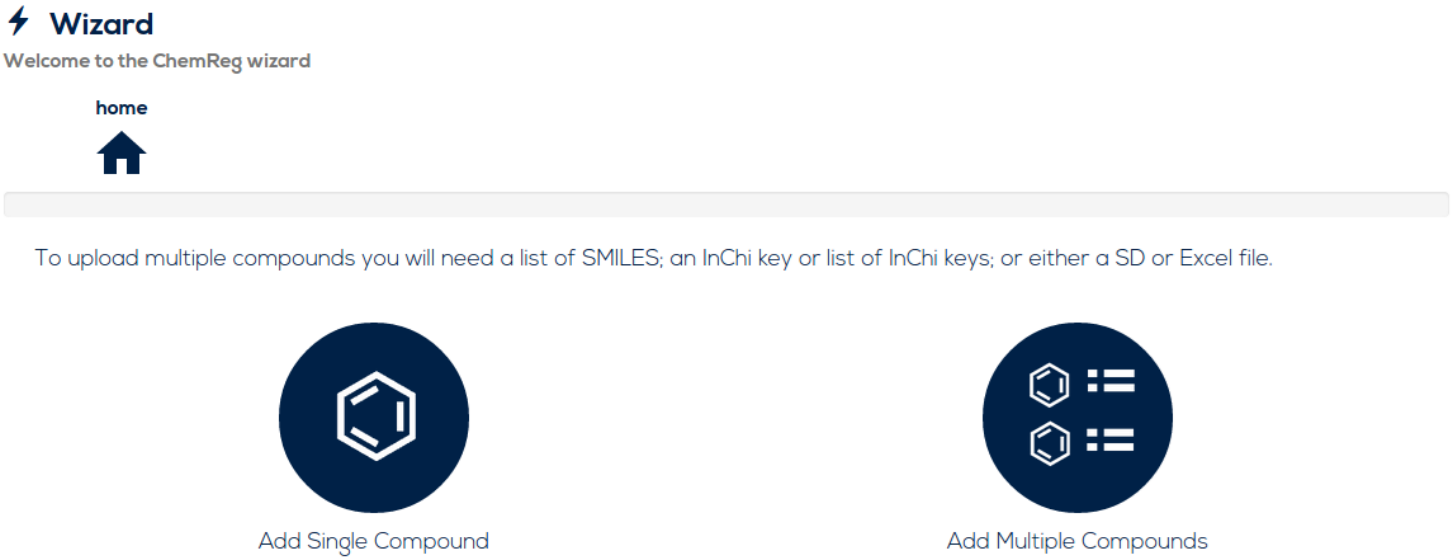






- Stereochemistry - same bond organisation but 3D differences
- Tautomeric forms - interchangeable structures e.g. ketones and enols
- “Batches” - structural information exists already but “real world” data is different, for example commercial supplier, purity.
- Pan Assay Interference (PAINS) compounds may be less desirable to register for some but not others
- Private vs Public compounds
- Blinded / Virtual compounds - do not initially have a structure

**All of these issues mean you can’t just “put” your compounds in a database with a generated ID.**

# Registration process




Chemical input wizard walks chemists through the process of registration

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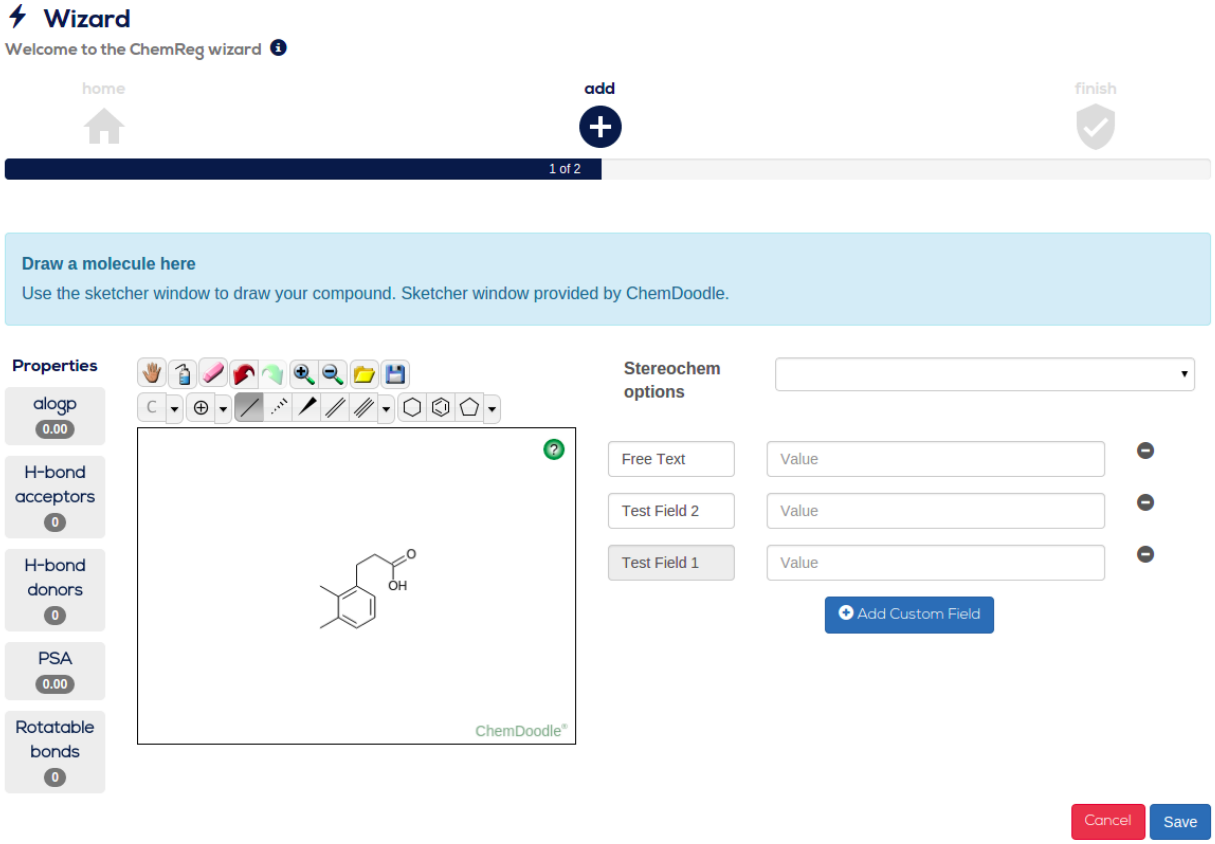
ChemBio Hub

# Registration process

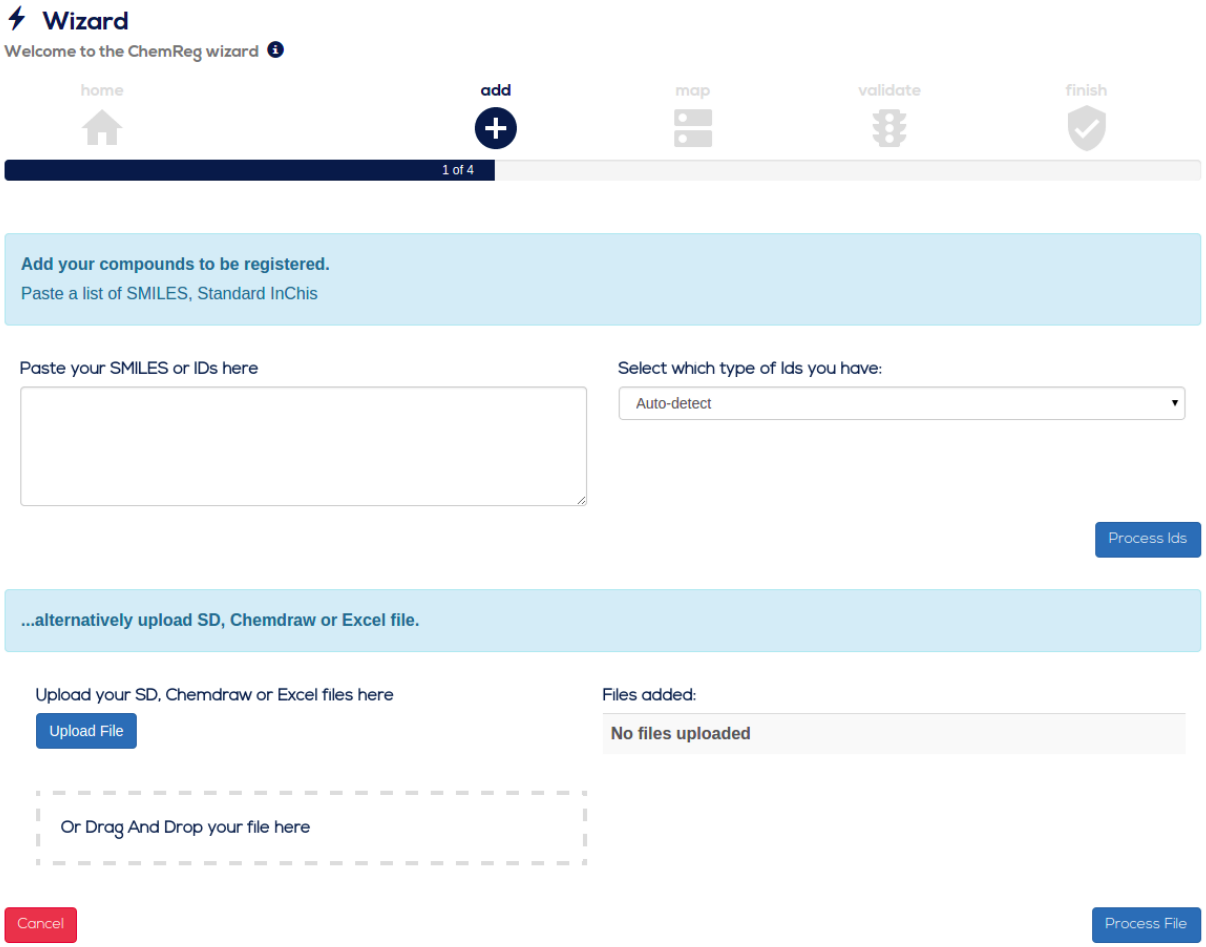



Users can sketch their molecule.

Live calculation of chemical properties gives feedback about the nature of the structure.

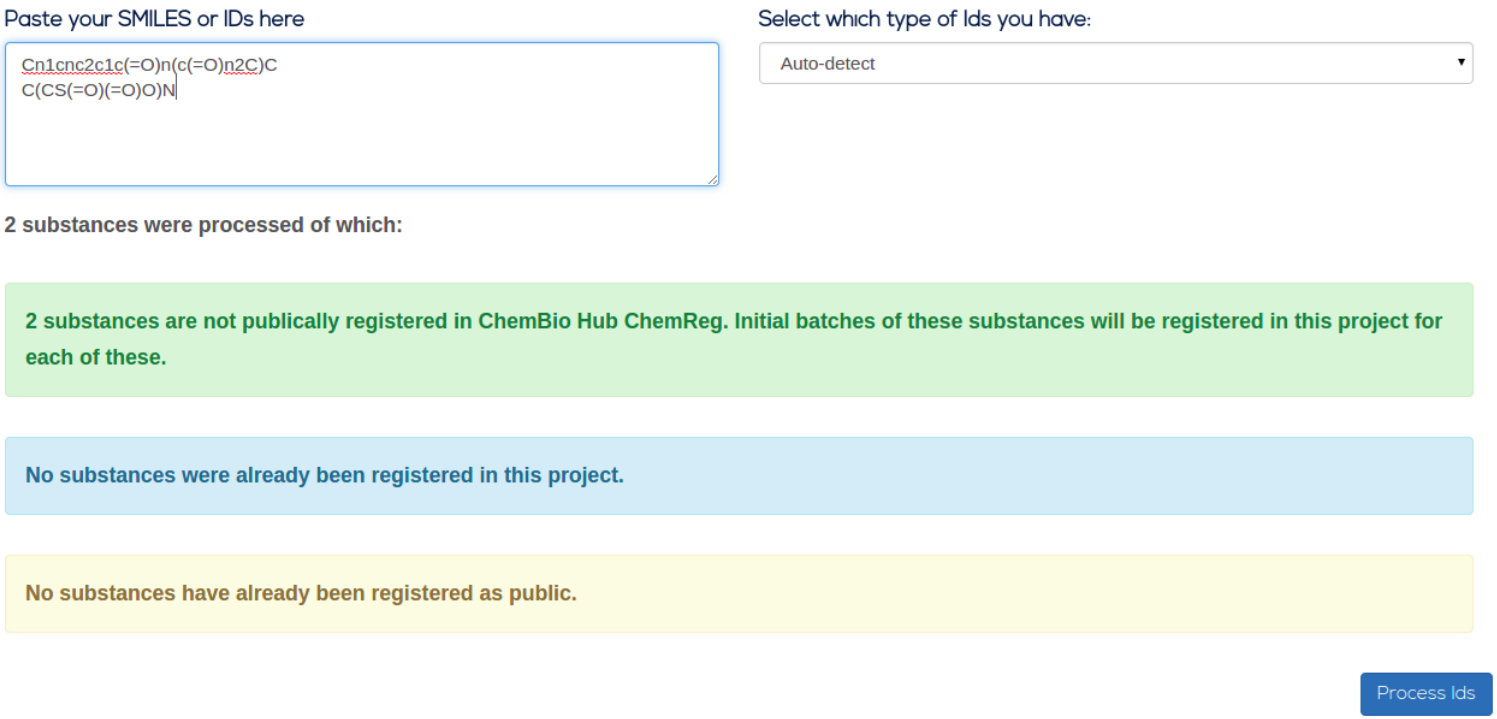
Users can add extra custom data to their registration

# Registration process



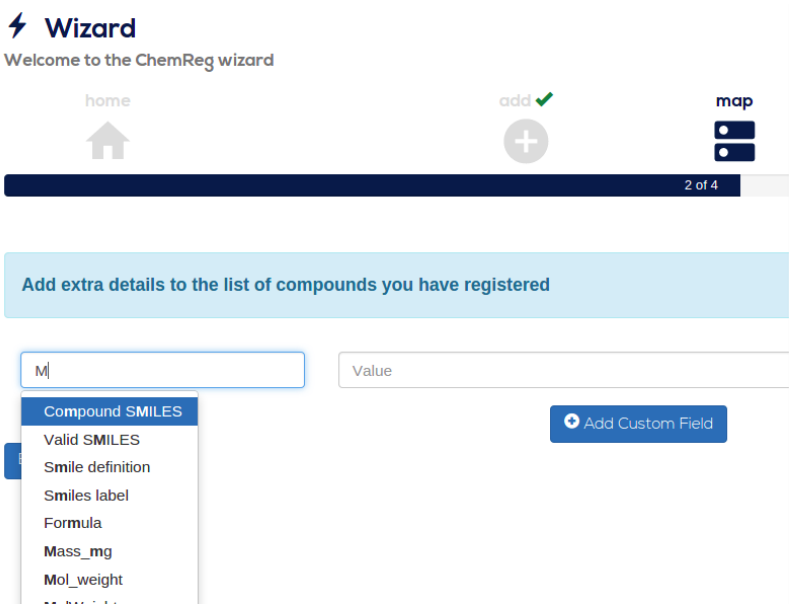

Users can add SMILES strings or InChi keys (text-based chemical structure representation) or in standard format files (SDF, ChemDraw or Excel)

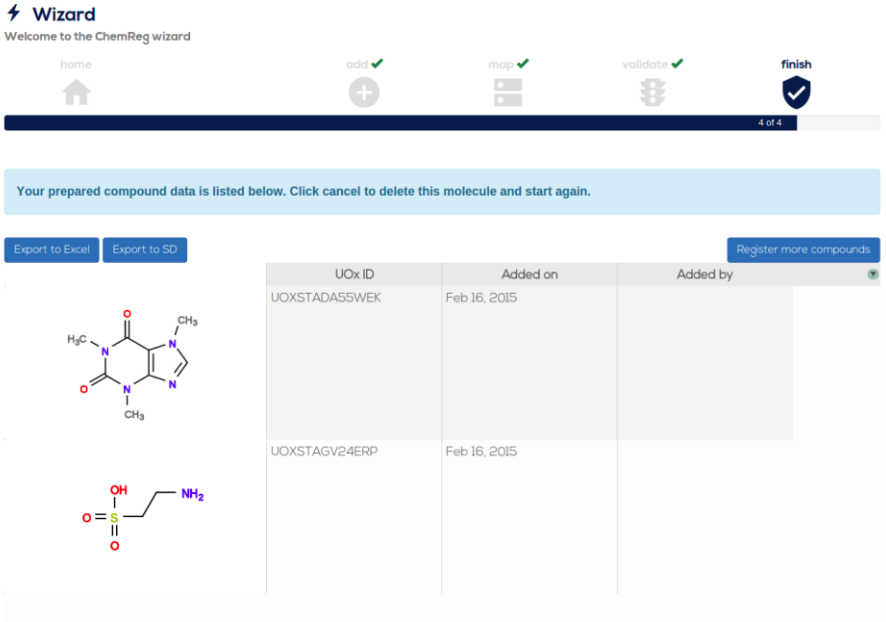
# Registration process




Active validation at every step
Information about what is currently in the database - overlaps
Problems and issues can be identified early in the process

# Registration process




Users can add extra custom data relevant to their project
Individual projects can make certain data fields mandatory
Results can be exported as SD or Excel file for auditing etc.

But it isn’t just about whizzy tools…

# There's some cool technology involved...

But they don't and won't define a successful project.

The aim is to:

- Change **how** researchers work for the better.
- So let's talk about **Knowledge Exchange**...
  - Working with Business Development, ISIS, the KE community and Pharma/Biotech

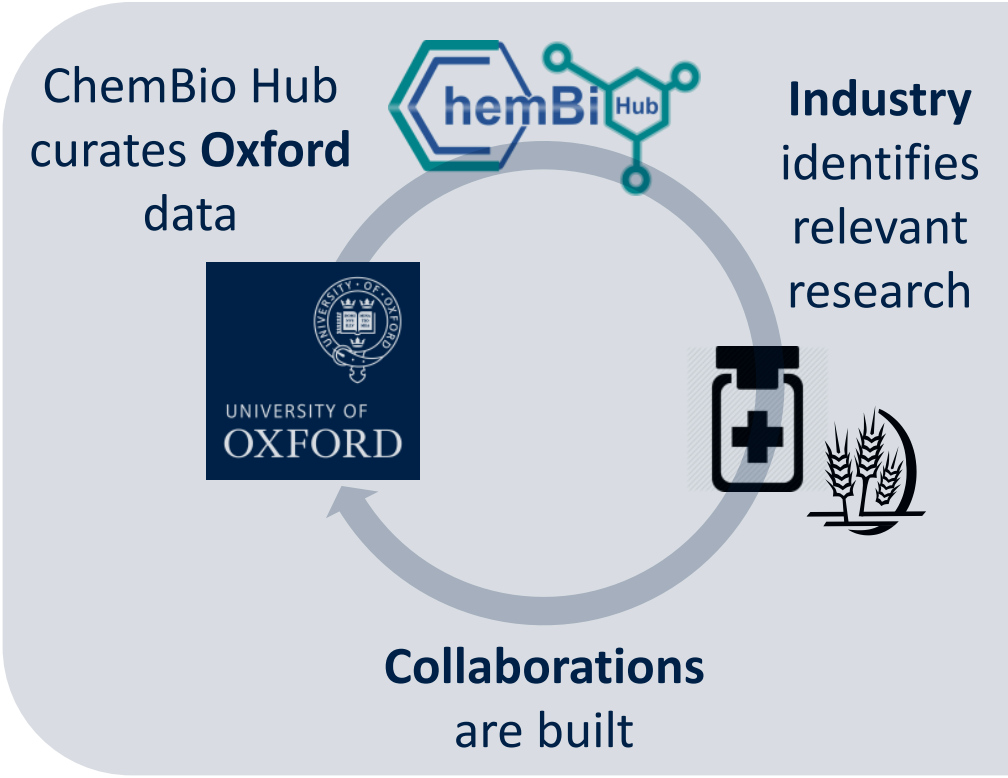
# People *as well as* data

- Great data management is just the beginning…
  - Ultimately it is **people** we need to connect
  - So that existing data can be turned into new ideas

# Industry outreach

- Critical to engage pharma and biotech companies now

- Learn industry-grade data management
- Find out how to best present data to industry
- Obtain industry buy-in to sustain ChemBio Hub




- Chicken & Egg: challenge of conveying vision early-on

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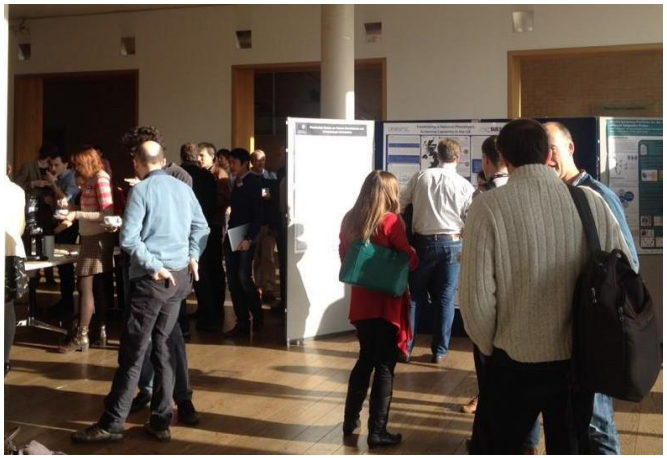
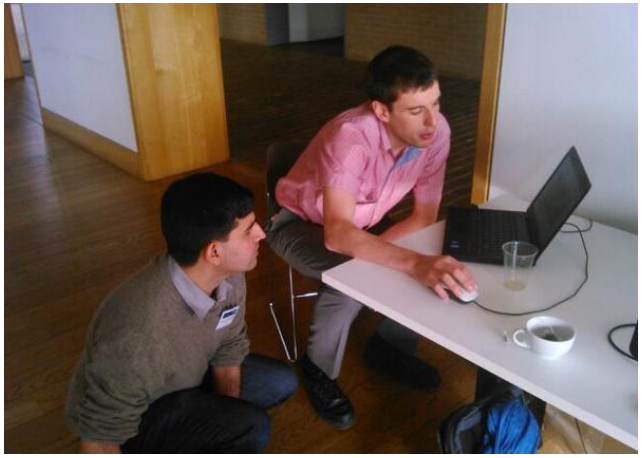
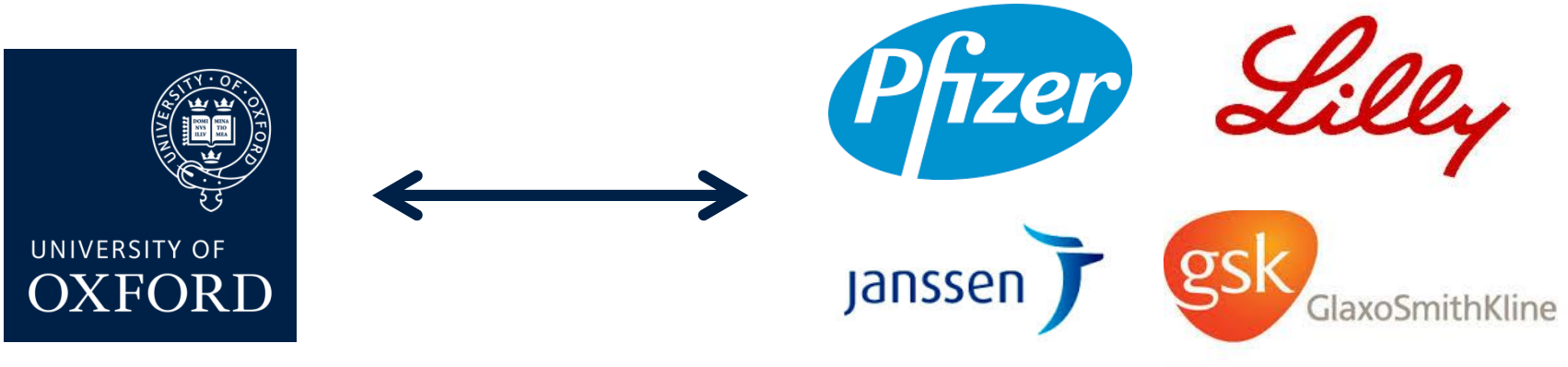
# People *as well as* data

- ChemBio Hub **Oxford** symposium – November 2014
- 100 Oxford researchers met and made new cross-departmental connections
- Generated 17 new collaboration ideas
- Live demos of ChemBio Hub data management tools





# People *as well as* data




- ChemBio Hub **Oxford-industry** symposium – July 2015
- Showcase Oxford capability to pharma and biotech groups
- Spark connections, conversations and collaborations
- Drive further industry funding of Oxford research

# What's next?

# Right now

We're recruiting pilot testers from multiple departments to prove the value of ChemBio Reg

- Chemistry
- DPAG
- Biochem
- WIMM
- Physics
- SGC
- TDI
- Pharmacology

And we're thinking about how to tackle Assay Capture

# What happens next?

- We have a year to develop code:
  - Registration of compounds
  - Assay definition
  - Assay results
- Keeping usability as a high priority
- Integrating with other systems
- Promoting collaboration and good data management
- Building the community

# And then..

- This is a permanent fixture, so it needs a support and growth plan. Multiple options:
  - Professional open source
  - Industry angels
  - Licence
  - Public funding
  - Other flavours and combinations

- We will explore these possibilities and more…

# Key Lessons

- You must fully understand the nuances of the data and its metadata before you dive in
- Engaging with users early is key – a technical solution that no one uses is a waste of time
- Keep your technology stack nimble, but don't box yourself into a corner with cool toys
- Cultural change is hard (no surprise!)
- Inspiration can come from very unlikely places

- You can build an awesome solution, but that does not guarantee sustainability

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ChemBio Hub

# Acknowledgements

http://chembiohub.ox.ac.uk

## The ChemBio Hub Team


Karen


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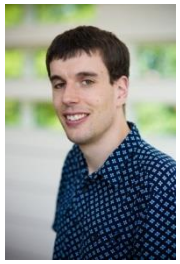
Andy


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## The SGC

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