



# PSDI

PHYSICAL SCIENCES  
DATA INFRASTRUCTURE

## Seekest thou the road to, all that's digital and FAIR – the Ballad of the ELN Journey

Please use the Q&A feature if you have a question during this webinar and we will answer them at an appropriate time

PSDI Webinar

14<sup>th</sup> August 2025

Dr Samantha Pearman-Kanza  
University of Southampton

<https://www.psd.ac.uk/>

# Presentation Outline

- ▶ About Me
- ▶ Why are we here?
- ▶ The Twisty Turny ELN Journey
  - ▶ Research
  - ▶ Challenges & Considerations
  - ▶ Case Study Learnings
- ▶ Relevant PSDI Resources



I'm here to keep her in line!

Now remember...you  
promised not to sing!



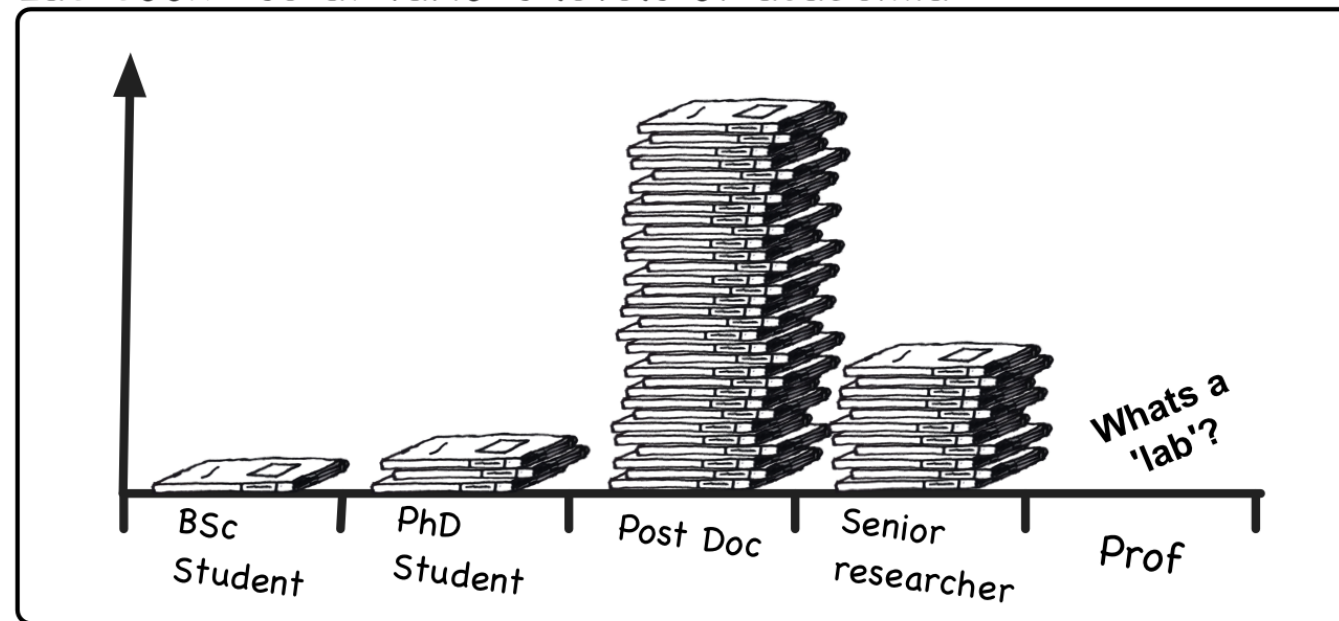
# About Me

- ▶ Computer Scientist turned Web Scientist masquerading as a Chemist
- ▶ Principal Enterprise Fellow at University of Southampton
- ▶ Principal Investigator for CaSDaR (Careers & Skills for Data-driven Research)
- ▶ Pathfinder Lead on Process Recording for PSDI (Physical Sciences Data Infrastructure)
- ▶ Lab Horizons Columnist: CompSci Cat
- ▶ Advisory Boards/Committees: Future Labs Live, London Labs Live, MADICES, , Machines Learning Chemistry, RSC-CICAG, STRIX Award, KnowLedger: An Open Digital Research Notebook for Research Data Management
- ▶ Research Interests: Data Stewardship, FAIR Data, Semantic Web Technologies, IoT, Research Data Management, Digitisation, Lab of the Future, Paperless Labs, Re-use of Technology

# Why are we here?

- ▶ Many scientific researchers have a fragmented paper/digital approach to writing up their experiments
- ▶ Research and data generation is being wasted due to these issues as people cannot access or build on others work
- ▶ Consequently, a vast quantity of scientific research cannot be re-used or reproduced

Lab book use at various levels of academia

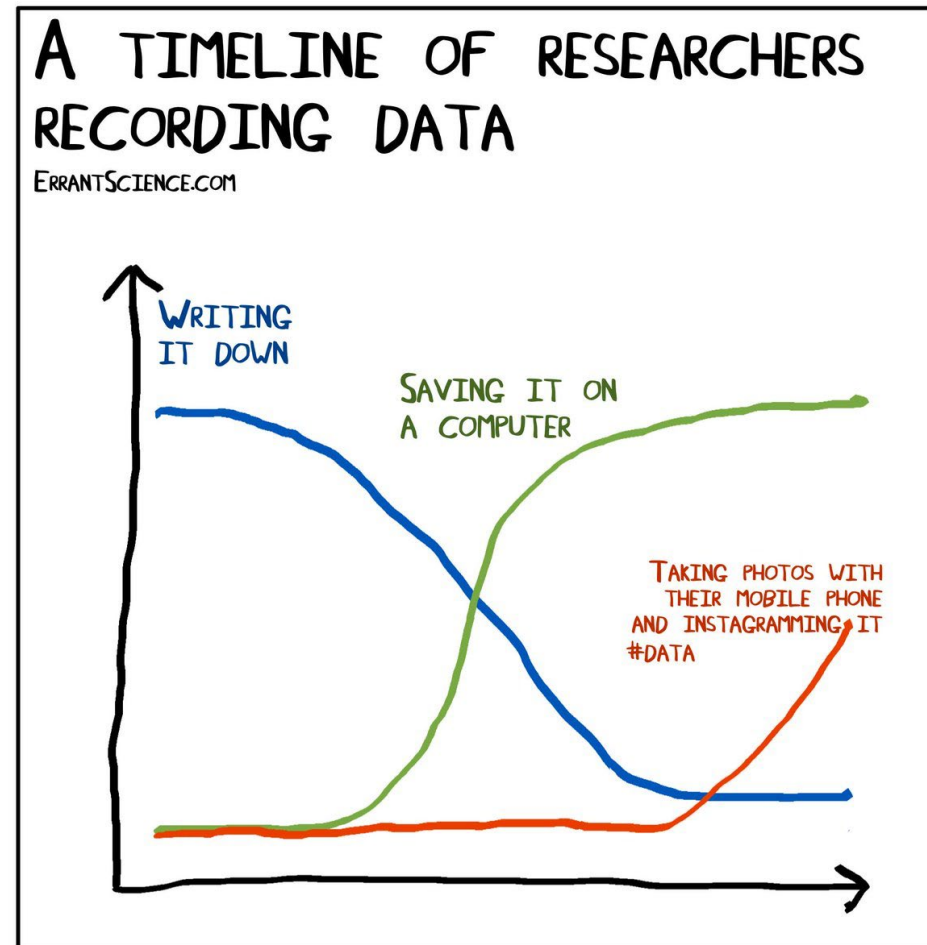




# So is paper the root of all evil?



- ▶ Not necessarily!
- ▶ Paper records aren't always bad e.g. Darwin's early Notebooks
- ▶ Electronic records / methods aren't always good e.g. spreadsheets with unintelligible column names
- ▶ Just because something is in an electronic form does not immediately make it high quality data!



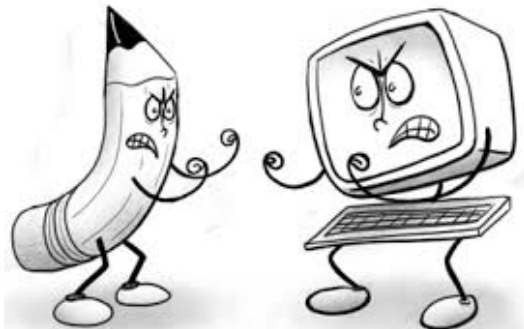
# Consequences of paper (or poor electronic sharing...)



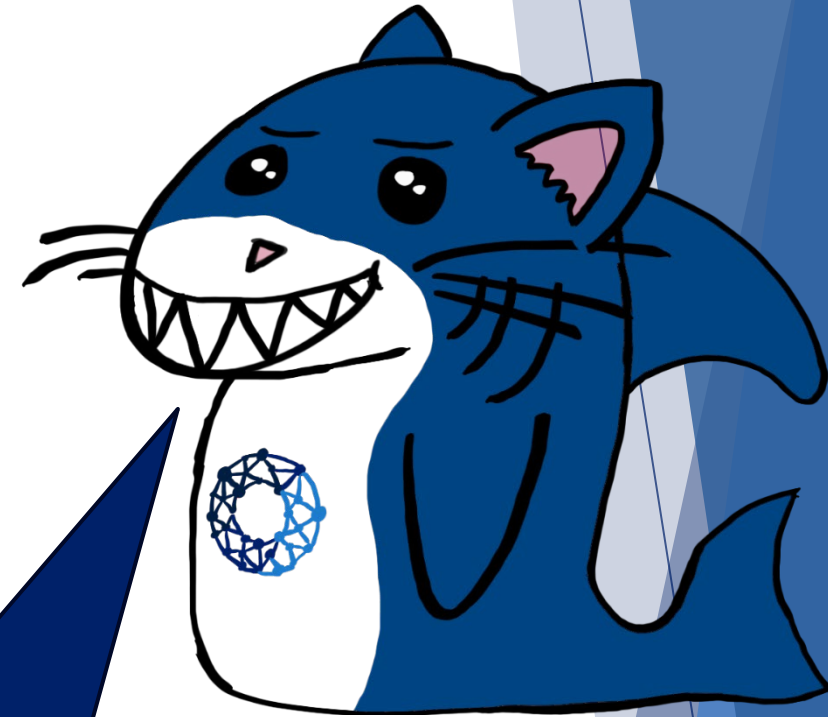
Cartoon drawn by Dr Cerys Willoughby for Kanza, S., Willoughby, C., Gibbins, N., Whitby, R., Frey, J.G., Erjavec, J., Zupančič, K., Hren, M. and Kovač, K., 2017. Electronic lab notebooks: can they replace paper?. Journal of cheminformatics, 9(1), p.31. <https://doi.org/10.1186/s13321-017-0221-3>

# Therefore...

- ▶ Ultimately, we should be moving towards maintaining electronic records because they are:
  - ▶ Easier to share
  - ▶ Easier to search
  - ▶ Easier to backup
  - ▶ Accessible from multiple locations



Move over Pencil! Sounds like we need some sort of Electronic System...



# Digital tools should enable

- ▶ Capturing data in a more structured form to improve quality
- ▶ Improved capability to search for and find your own work
- ▶ Better sharing between researchers
- ▶ Preservation of valuable research for future use
- ▶ Production of FAIRer data for publication
- ▶ ELNs are a potential solution to this!



[“Electronic Lab Notebooks are great, but not on vacation”](#) Cartoon by Phil Johnson for MIT.

# PhD Research (2014-2018)



”What do you mean people are still using paper?! Surely this ELN thing is just THE ANSWER.....I’m sure it’s a simple solution....”

*Samantha Kanza, 2014*

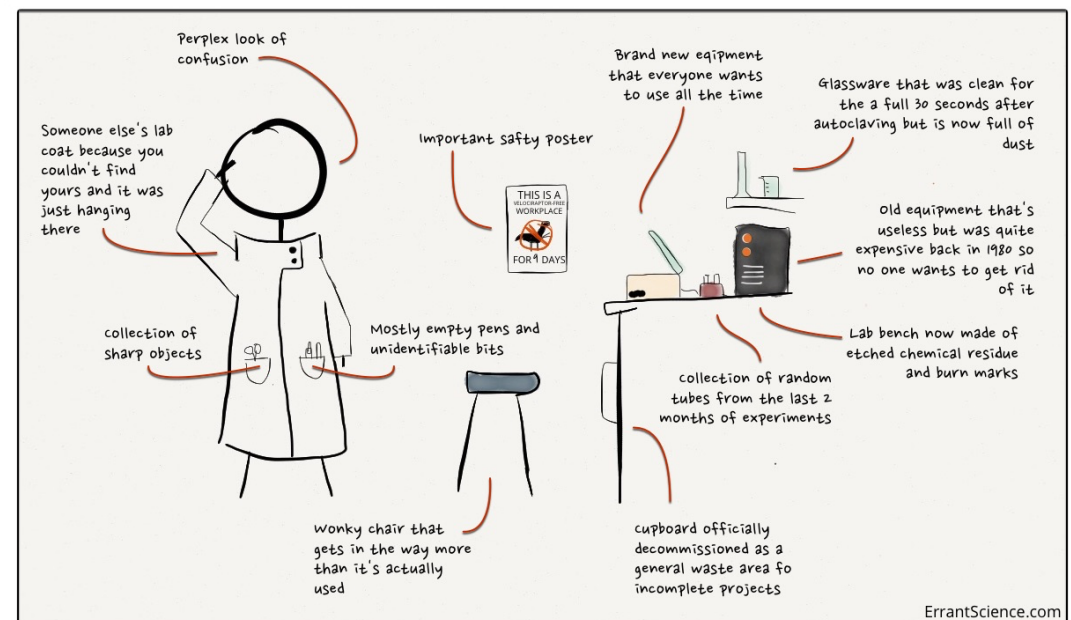


Foolish  
Mortal!



# Into the Field (2014-2018)

- ▶ **ELN Landscape Research** – Understand current state of the market for ELNs
- ▶ **Surveys and Focus Groups** – ascertain current lab practice with physicists/biologists/chemists
- ▶ **Lab Observations** – observe lab environment (Inorganic Chemistry, Organic Chemistry, Molecular Chemistry, Crystallography)



A guide to a typical research lab

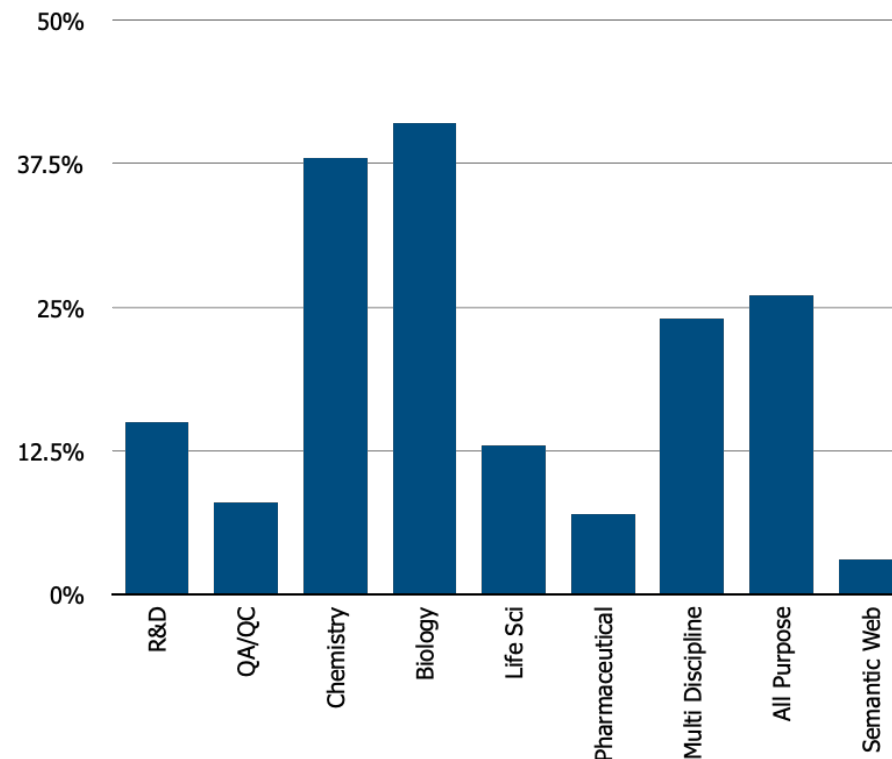
["A guide to a typical research lab"](#) by ErrantScience.com is licensed under [CC-BY-NC](#)

# The Saturated Market 2018

ELN Licenses		
License	Total	%
Commercial	77	86.52%
Open Source	9	10.11%
Free Version	14	15.73%
ELN Platforms		
Platform	Total	%
Independent	48	53.93%
Web Based	40	44.94%
Windows	28	31.46%
Mac	16	17.98%
Unspecified	11	12.36%
Other Software	8	8.99%

Active/Inactive ELNS			
	Active	Inactive	Total
ELNs	88	34	122

**Distribution of ELN Domain Representation in 2018**



# Barriers to Implementation/Usage (2018)

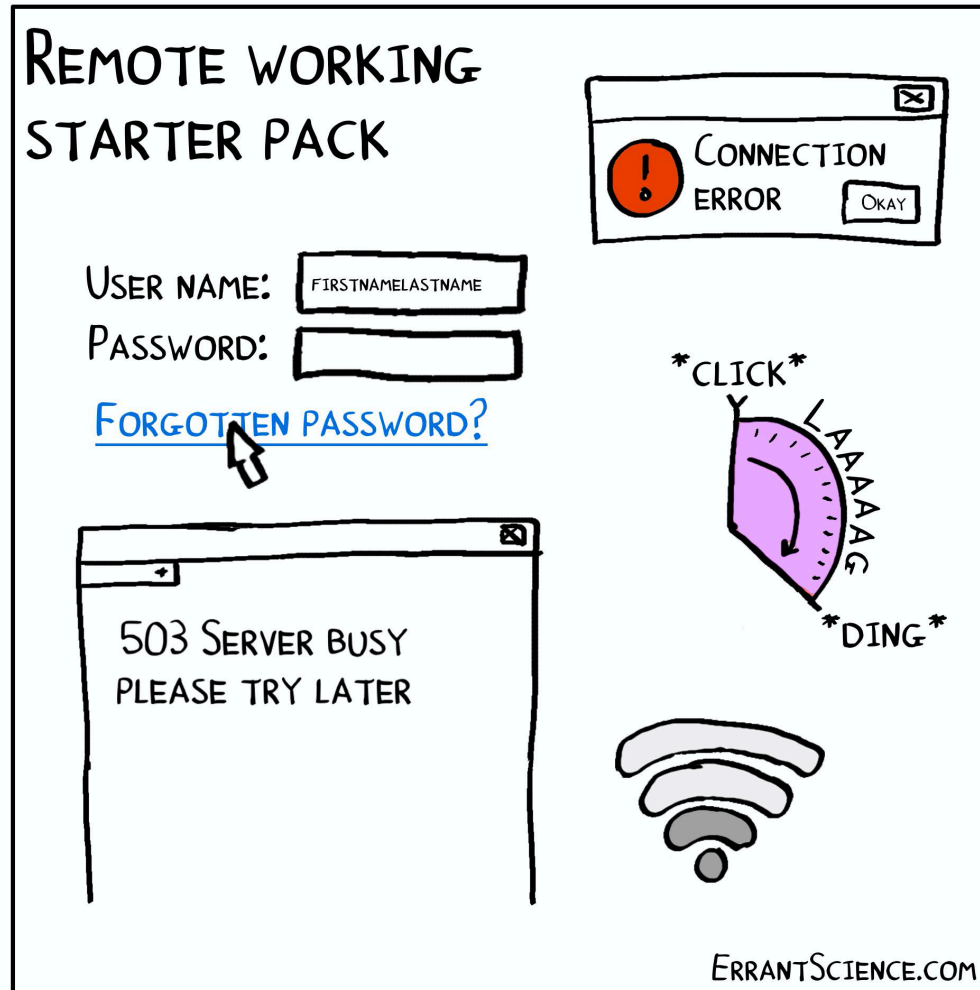
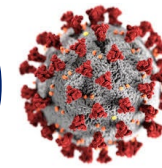
Category	Barriers	% of 169
<b>Accessibility:</b> Use in and out of the lab	You'd need to enter data in both the lab and write-up area	74
	No easy access to appropriate hardware in the lab	12.5
<b>Ease of use:</b> Not as easy as paper	ELN was too difficult to use	22
	Des not capture the right information for me	7
	Difficult to capture some kinds of information in an ELN	80
<b>ELN attitude:</b> Requires change of attitude from higher ups / from the onset	Only makes sense if the whole department adopts it	20
	Belief that students/post docs would resist adoption	11
<b>Cost:</b> People don't want to pay	Up front costs and licensing fees	74
	Additional infrastructure costs (e.g. computers)	27
	Future development and costs of applications	90
	On-going costs of the system	93
<b>Data Portability:</b> Data can't always be moved between notebooks or machines	Data will be tied into a commercial package	84
Other	Other	11

- ▶ Logistical Barriers
- ▶ People Barriers
- ▶ Data Barriers
- ▶ Hardware Barriers
- ▶ Software Barriers

## ▶ Environmental Barriers

- ▶ Hostile Lab Environment (Chemicals, Magnetised Equipment)
- ▶ Limited Space for Laptops

# Fast forward to 2020



"Remote working starter pack" by ErrantScience.com is licensed under [CC-BY-NC](https://creativecommons.org/licenses/by-nc/4.0/)

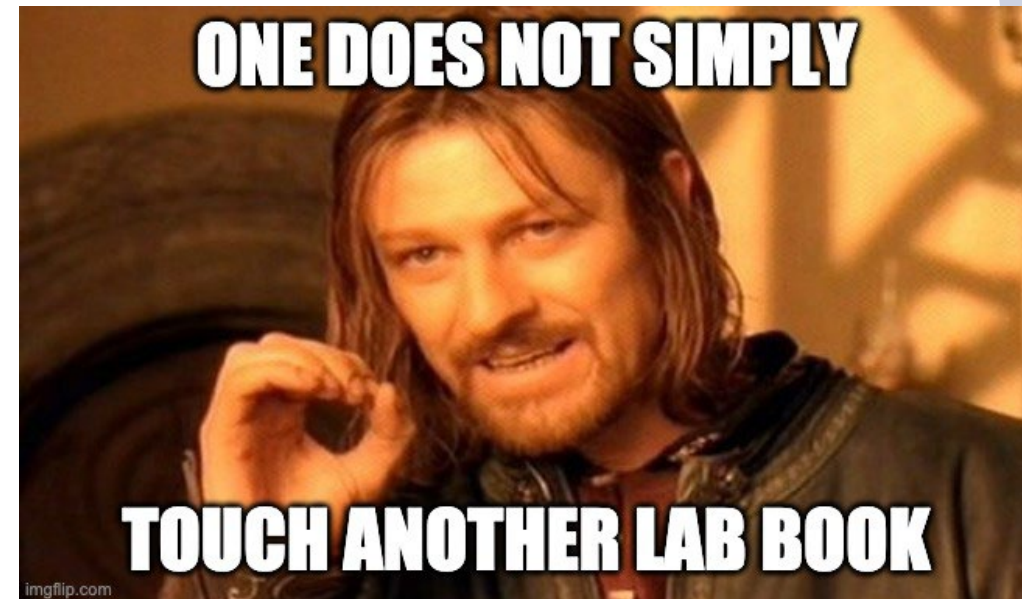


Image created using: <https://imgflip.com/memegenerator/>

# Fast forward to 2021

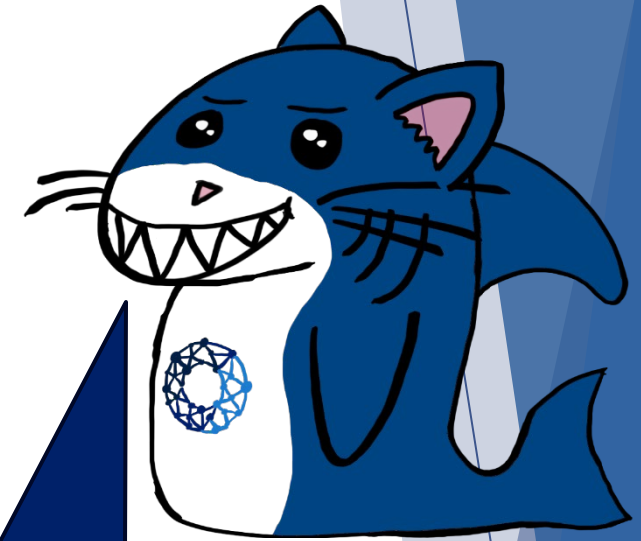
Everything  
has changed!

Or has it...?

Yes & No...



Image taken from: <https://www.giantfreakinrobot.com/ent/tardis-doctor-who.html>



Helpful...



# PSDI Pilot Study & Phase 1 Work (2021-2023)

- ▶ Systematic Literature Review
- ▶ Investigation of Tools and technologies available to the Physical Sciences
- ▶ Survey to ascertain if the current landscape had changed, and what the Physical Sciences community needs
- ▶ Survey to establish current ELN Usage and requirements



Obviously all  
masterminded  
by me

# State of Play (2022-2023)

## USE OF PAPER VS ELECTRONIC

### Similarities

- Researchers still work in different ways using a mix of paper/electronic methods
- Paper still more used for planning, with a heavy reliance on computational methods for analysis and writeup

### Differences

- Reduction in only using Paper



## ORGANISING & LINKING WORK

### Similarities

- Necessity to link between paper and electronic demonstrates a use of paper
- Still a clear pattern of using codes/links to bridge this gap

### Differences

- Increase in software to organise and link work



## BARRIERS TO DIGITAL RESEARCH

- Logistical Barriers (*Cost, Time*)
- People Barriers (*Unwilling to adopt, Training*)
- Data Barriers (*Data Import/Export issues, Archiving, Data Integration*)
- Hardware & Software Barriers (*Storage, Hardware & Software Interoperability, Links between software packages*)

Much the same as 2018



## USE OF A DIGITAL NOTEBOOK/ELN

In our 2021 Survey 55% said YES to using a Digital Research Notebook (note that is not necessarily an ELN)

In our 2022 Survey 50% said NONE to what ELN do you use, with 17% using Generic Notebooks and 33% using 17 Different ELNs



## EVOLUTION OF ELNS

- Many different terms for ELN “Digital Research Platform, ERN, RDM Software”
- Platforms now exist that encompass
  - ELNs (Electronic Lab Notebooks)
  - LIMS (Laboratory Information Management System)
  - SDMS (Scientific Data Management System)
  - Inventory / Sample Management
- NOT JUST A REPLACEMENT



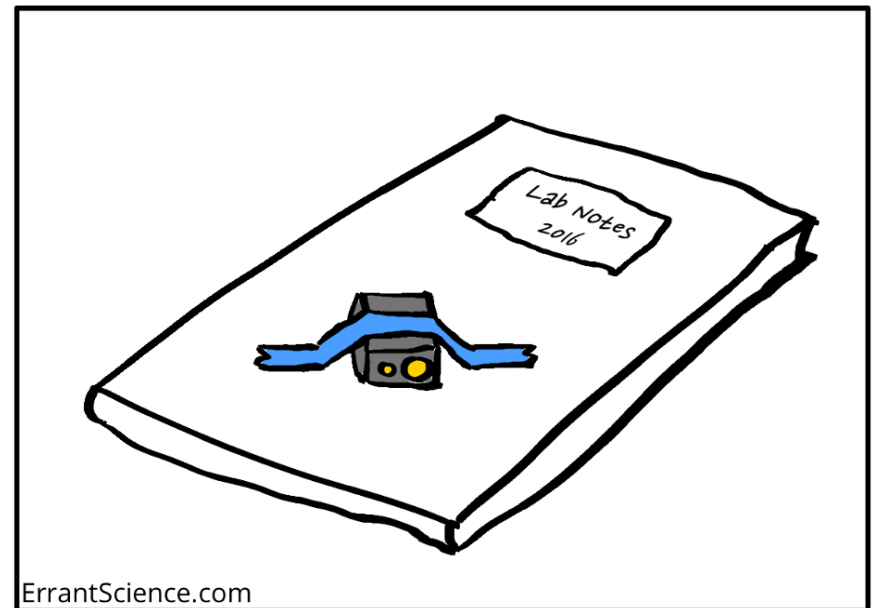
## SATURATED MARKET

- There are still over 80 active ELNs on the Market



# PSDI Process Recording Case Studies

- ▶ Case studies of implementing different Process Recording Systems
  - Generic Notebook Implementation
    - University of Nottingham – OneNote in Chemistry Teaching Labs
    - University of Southampton – OneNote in Chemistry Teaching Labs
    - Wellington College – OneNote in School Labs across Chemistry, Physics & Biology
  - Open Source In House ELN
    - University of Nottingham - AI4Green in Undergrad & Postgrad Labs (Student Edition & Research Edition)
  - Large-Scale Commercial ELN
    - University of Southampton - Revvity Signals in the Postgraduate Labs across 12 different Research groups



If your electronic lab book looks like this,  
you're doing it wrong

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# Challenges & Considerations



Image created using imgflip.com

- ▶ Choice
- ▶ Time
- ▶ Infrastructure
- ▶ Data
- ▶ Cost
- ▶ People / Change Management

# Electronic Lab Notebooks



There are now over 85 active ELNs on the market!

- |                            |                       |                 |                              |
|----------------------------|-----------------------|-----------------|------------------------------|
| ▶ ACAS                     | ▶ Ec-LabNote          | ▶ LabFolder     | ▶ Online ELN Worksheet       |
| ▶ Active LN                | ▶ eLabFTW             | ▶ Labguru ELN   | ▶ Open Enventory             |
| ▶ AgiLab ELN               | ▶ eLabJournal         | ▶ Labii         | ▶ openBIS                    |
| ▶ Agilent SLIMS            | ▶ eLabNotes           | ▶ LabKey ELN    | ▶ OpenText ELN               |
| ▶ AI4Green                 | ▶ EmsoChemLab         | ▶ LabLog        | ▶ PASTA-ELN                  |
| ▶ Alchemy ELN              | ▶ Espresso ELN        | ▶ LabsForm      | ▶ PatentSafe ELN             |
| ▶ Arxspan ELN              | ▶ eStudy              | ▶ LabSpace      | ▶ quattro/LJ                 |
| ▶ Benchling ELN            | ▶ eSystems            | ▶ LabStep       | ▶ RedFox                     |
| ▶ BioChemLab Solutions ELN | ▶ Formulator          | ▶ LabTrack ELN  | ▶ Rspace                     |
| ▶ BioRails                 | ▶ Gene Inspector      | ▶ LabTrove      | ▶ SampleDB                   |
| ▶ Biovia Notebook          | ▶ GenoFAB             | ▶ LabVantage    | ▶ Sapio Seamless ELN         |
| ▶ Bookitlab                | ▶ GOLims              | ▶ LabWare ELN   | ▶ SciCord ELN/LIMS           |
| ▶ CBIS E-Notebook          | ▶ Herbie              | ▶ Laby          | ▶ Sciformation ELN           |
| ▶ CDD Vault ELN            | ▶ iLES Platform       | ▶ Limsophy LIMS | ▶ Sciligence ELN             |
| ▶ CERF 5.0                 | ▶ InELN               | ▶ LogBook       | ▶ SciNote                    |
| ▶ ChemCart ELN             | ▶ iQ                  | ▶ Logilab       | ▶ Signals ELN                |
| ▶ Chemia                   | ▶ Kadi4Mat            | ▶ LOGS-ELN      | ▶ Stackwave ELN              |
| ▶ Chemotion                | ▶ Lab Integrated Data | ▶ Mbook         | ▶ STARLIMS ELN               |
| ▶ Colabra ELN              | ▶ (LabID)             | ▶ MyLabBook     | ▶ Studylog                   |
| ▶ CompuDrug ELN            | ▶ LabArchives         | ▶ NOMAD ELN     | ▶ Sun Bio ELN                |
| ▶ Dotmatics ELN            | ▶ LabCloud            | ▶ NotebookMaker | ▶ Thermo Scientific Core ELN |
| ▶ E-WorkBook               | ▶ LabCollector ELN    | ▶ NuGenesis     | ▶ Unaccountable              |



# Generic Notebooks

## Note-Taking Apps

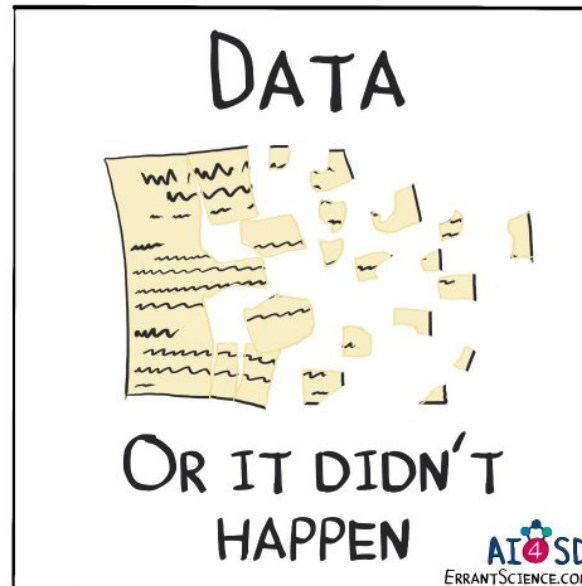
- ▶ Apple Notes
- ▶ Evernote
- ▶ GoodNotes app
- ▶ Google Keep
- ▶ Joplin
- ▶ Notability
- ▶ Notion
- ▶ OneNote
- ▶ Simplenote
- ▶ Obsidian
- ▶ Zim

## Word Processors

- ▶ Apple Pages
- ▶ Google Docs
- ▶ Libre Office Writer
  - ▶ MS Word

## Text Editors

- ▶ Emacs
- ▶ Notepad
- ▶ Notepad++
- ▶ Sublime
- ▶ TextEdit
- ▶ Vi
- ▶ Vim



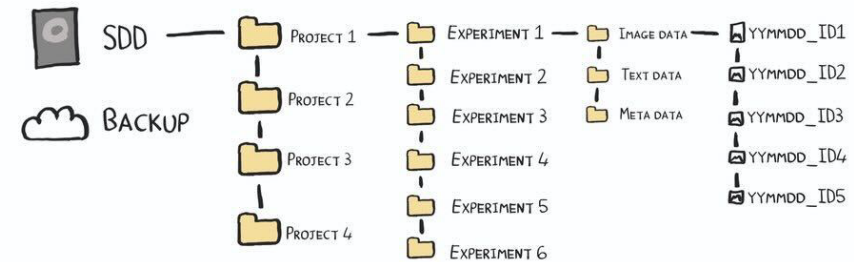
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# Choice Considerations



- ▶ Digitising is great, but WHY are you doing it?
- ▶ What data are you recording? How? Where?
- ▶ What data is not being recorded?
- ▶ What are the actual pain points that you are trying to solve?
- ▶ Does the software align with what you are trying to achieve?
- ▶ Implementing Digital Notebooks isn't just about the software, is your entire plan/setup moving towards your goal?

## How DATA SHOULD BE ORGANISED



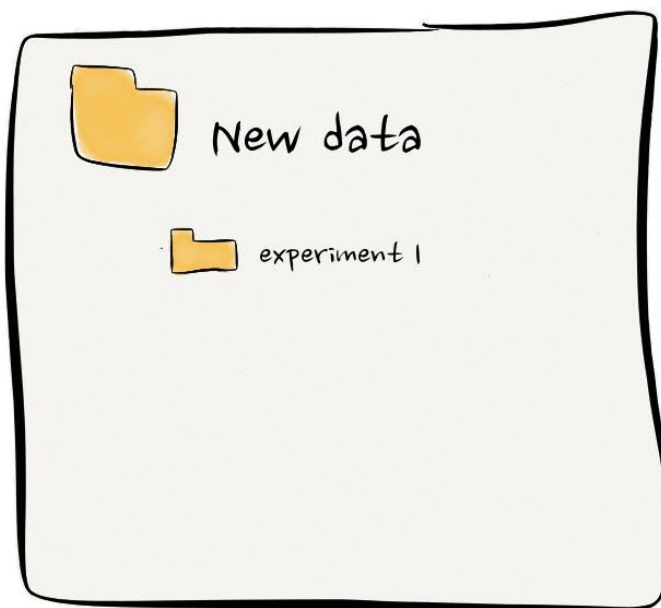
## How MOST DATA IS ACTUALLY ORGANISED



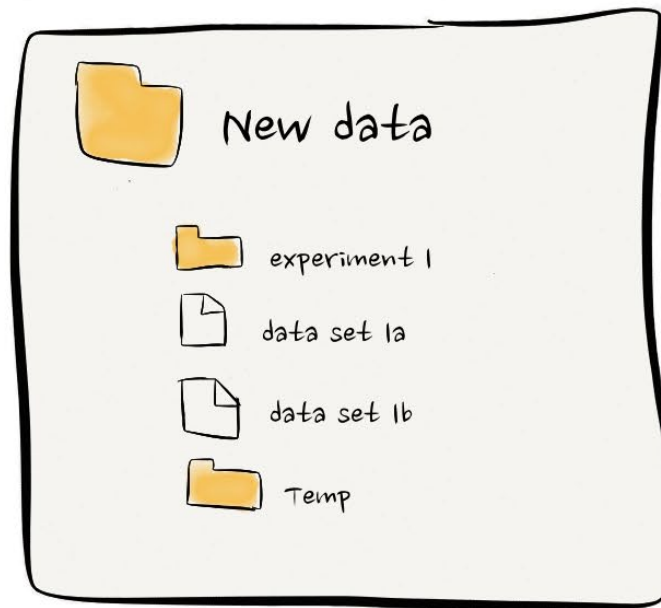
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# Domain Consideration

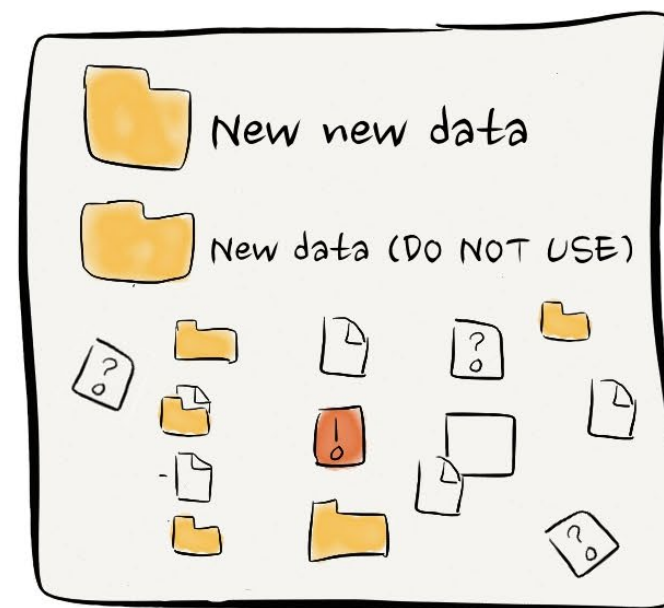
- ▶ Different domains have different requirements and data types
- ▶ Universities (and many companies) will need to cater for a variety of domains
- ▶ Finding one ELN for your entire institution is unlikely



**Day 1**



**Day 2**

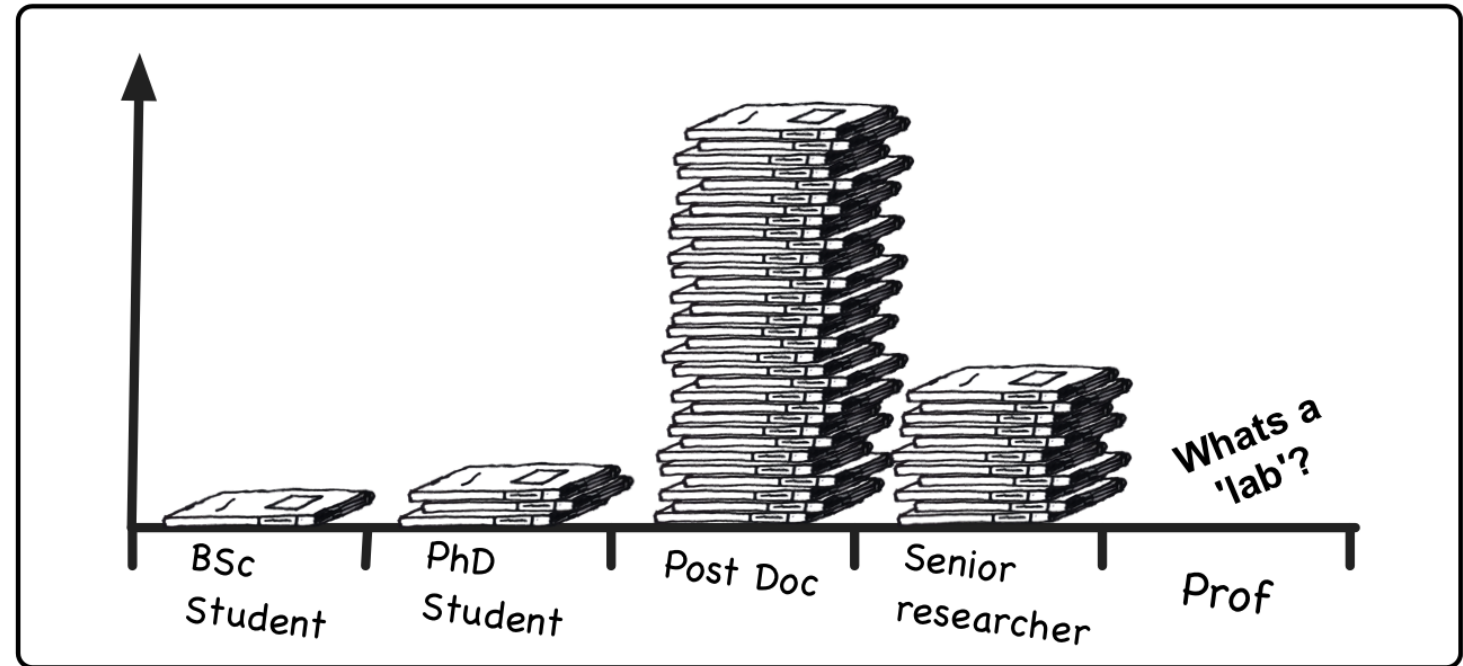


**Day 3**

# Career Level Consideration

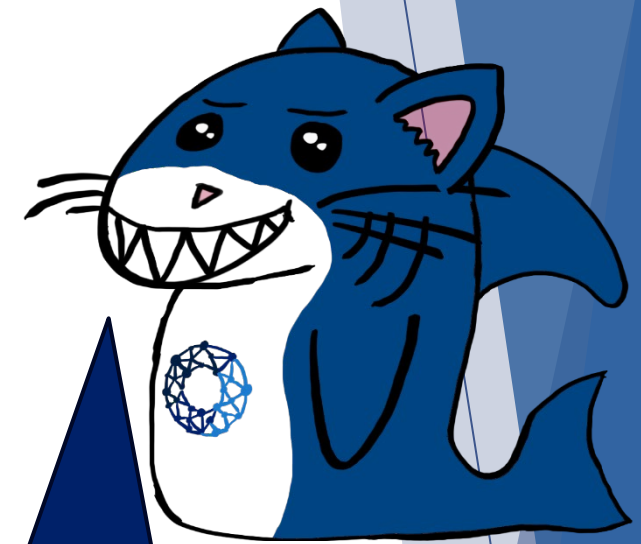
- ▶ Different career stages can have different needs from Digital Notebooks
- ▶ Undergraduate tools need to facilitate learning – are closed formats an issue here?
- ▶ Postgraduate/Industry tools need to enable the capture and production of FAIR data
- ▶ Important questions
  - ▶ How automated do you want/need this ELN to be?
  - ▶ Is a fully fledged ELN or a Generic Notebooking tool more appropriate?

Lab book use at various levels of academia



# Case Study Learnings

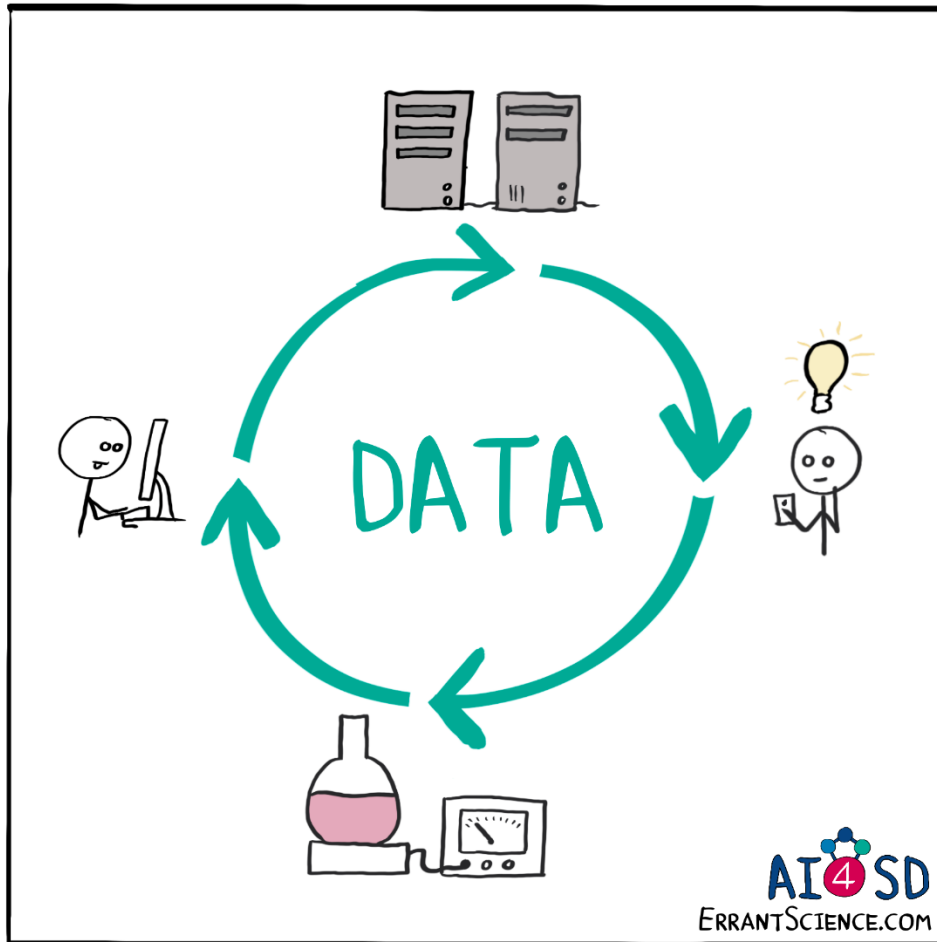
- ▶ **Generic Notebook Tool**
  - ▶ Selection of simple notebooking tool to replace paper
  - ▶ Chose a known tool already implemented in the current ecosystem
- ▶ **AI4Green**
  - ▶ Creation of a two new ELN Tools (Pedagogical Version for Teaching, Research Version for Researchers)
- ▶ **Revvity Signals**
  - ▶ Selection of a large-scale ELN tool that could meet the needs of different subdomains of Chemistry
  - ▶ Chose a tool that is compatible with heavily used departmental software (ChemDraw)



There is no “right answer” (although there can be some wrong ones...), its more about HOW you implement it



# Infrastructure/Institutional Considerations



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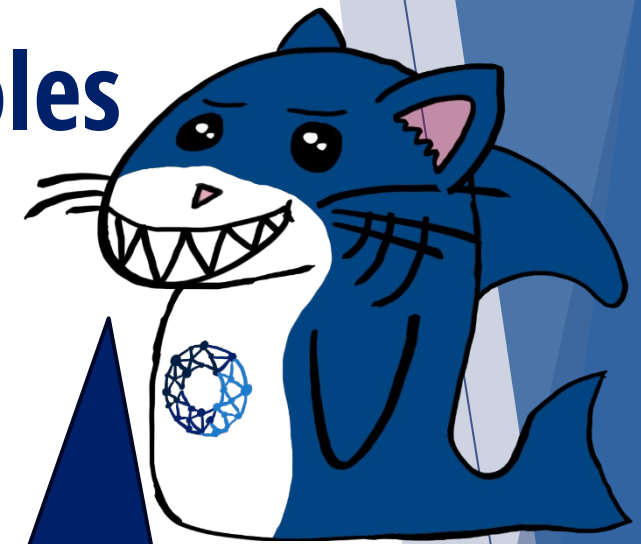
- ▶ Infrastructure Setup
- ▶ Stakeholders
- ▶ Finances
- ▶ Time
- ▶ Procuring Devices
- ▶ Environmental Setup

# Infrastructure / Administration



- ▶ ELN Implementation is more than just buying software licenses
- ▶ There are a range of stakeholders and roles to consider
- ▶ A solid infrastructure needs to be established for a successful implementation

# Identifying Stakeholders & Roles



## ► Stakeholders Types

- **Primary Stakeholders:** Direct Users of the ELN
- **Secondary Stakeholders:** Not primary users of the ELN, they support and have influence over its usage
- **Tertiary Stakeholders:** Provide supporting infrastructure to run the ELN

## ► Identifying Roles

- What people power and different roles do we need?

Where do I fit in?

# Stakeholders (Southampton – Revvity)

## PRIMARY STAKEHOLDERS

- **Researchers/Students:**  
*They will use the ELN on a day-to-day basis. They will use it to plan and record their experiments and be able to share their work with other researchers and their group leaders.*
- **Group Leaders:**  
*They will use the ELN regularly to oversee their researchers research activities, they will sign off experiments and ensure that their researchers are adhering to both best research practices and adhering to the relevant health and safety terms. They might also use the ELN to do their own research.*
- **Teaching Staff:**  
*They will use the ELN within their modules for students to record their lab work and project work.*

1

## SECONDARY STAKEHOLDERS

- **Head of Chemistry & Chemical Engineering:**  
*They sign off on the budget for the ELN, they will have influence over its adoption and how its implemented but won't necessarily use it on a day-to-day basis.*
- **Health & Safety Staff:**  
*They will review the Health and Safety documents within the ELN to ensure compliance, if there is an incident they will use the ELN to retrieve the relevant experiment and health and safety entries, and if there is an audit they will use the ELN to pull out all of the health and safety documents required.*

2

## TERTIARY STAKEHOLDERS

**ELN Administrators:**  
*They will oversee initial ELN development, creating and turning on features and templates, developing and running training, and supporting the users with any queries on how to use the system.*

**IT Support Staff:**  
*They will ensure the smooth running of the service from a technical perspective, they will work with the vendor to integrate single sign on and will run backup scripts to ensure all entries are backed up safely to the relevant University file store locations.*

**Administrative Staff:**  
*They will administer the user accounts and groups to ensure that the required individuals can access the relevant parts of the ELN.*

3

# Roles (Southampton Revvity)

## LOCAL ELN MANAGER

- Provide training for the new system
- Fix/address any bugs
- Point of contact for the school for queries
- Key contact with the vendor
- Handle License agreements/renewals
- Coordinate across different stakeholders



## TECHNICAL TEAM

- Run backup scripts daily & ensure security
- Facilitate access to backups where required

## ADMINISTRATIVE TEAM

- Administer User Groups
- Ensure researchers are added to the correct groups with relevant permissions
- Deactivate users and hand over accounts



## HEALTH & SAFETY TEAM

- Work with ELN Manager to ensure needs are being met and they have relevant access to documents
- Oversee inventory setup



## GROUP LEADERS

- Work with ELN Manager to ensure templates in the ELN are sufficient for their sub domains
- Decide on sharing levels for groups
- Oversee and sign off health and safety documents and experiments
- 



## RESEARCHERS/STUDENTS

- Be trained to use the new system
- Document their plans and experiments in the ELN
- Adhere to health and safety policies
- Send health and safety documents and experiments to group leader for sign off



## TEACHING STAFF

- Be trained to use the system
- Work with ELN Manager to incorporate ELN into Teaching Laboratories
- Work with ELN Manager to get relevant templates set up





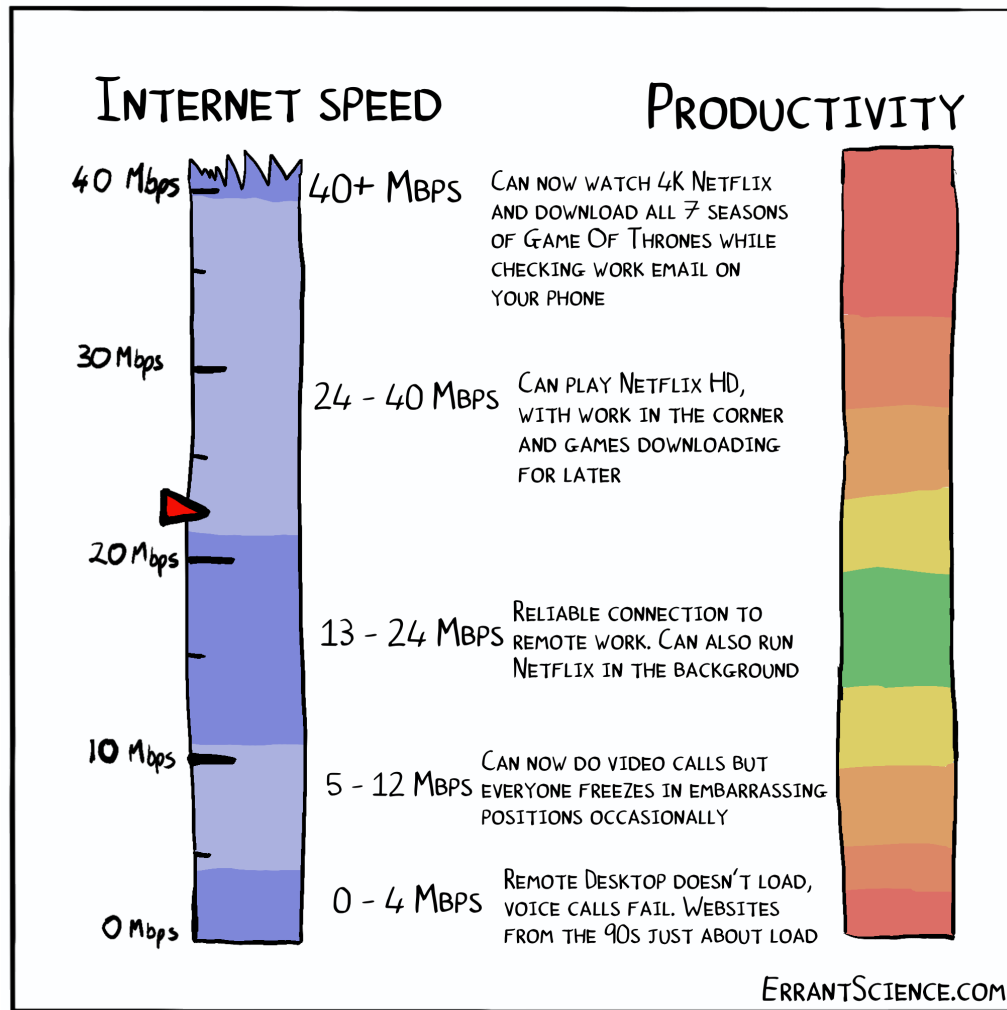
# Time Considerations



<https://www.pinterest.co.uk/pin/19281104642853801/>

- ▶ Implementing a new ELN takes considerable time
  - ▶ Time to convince people/institution
  - ▶ Obtain Budget Approval
  - ▶ Setup Lab suitably
  - ▶ Identify Staffing for admin/infrastructure
  - ▶ Run a trial
  - ▶ Develop templates
  - ▶ Organise logistics
  - ▶ Do not expect this to happen overnight!

# Hardware Barriers



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## Hardware Devices

- ▶ What electronic devices are going to be used?
- ▶ Are students expected to supply them themselves?
- ▶ Will staff need extra devices?

## Compatibility Concerns

- ▶ Will a Digital Notebook be interoperable with available (potentially legacy) hardware equipment ?

## Environmental Setup

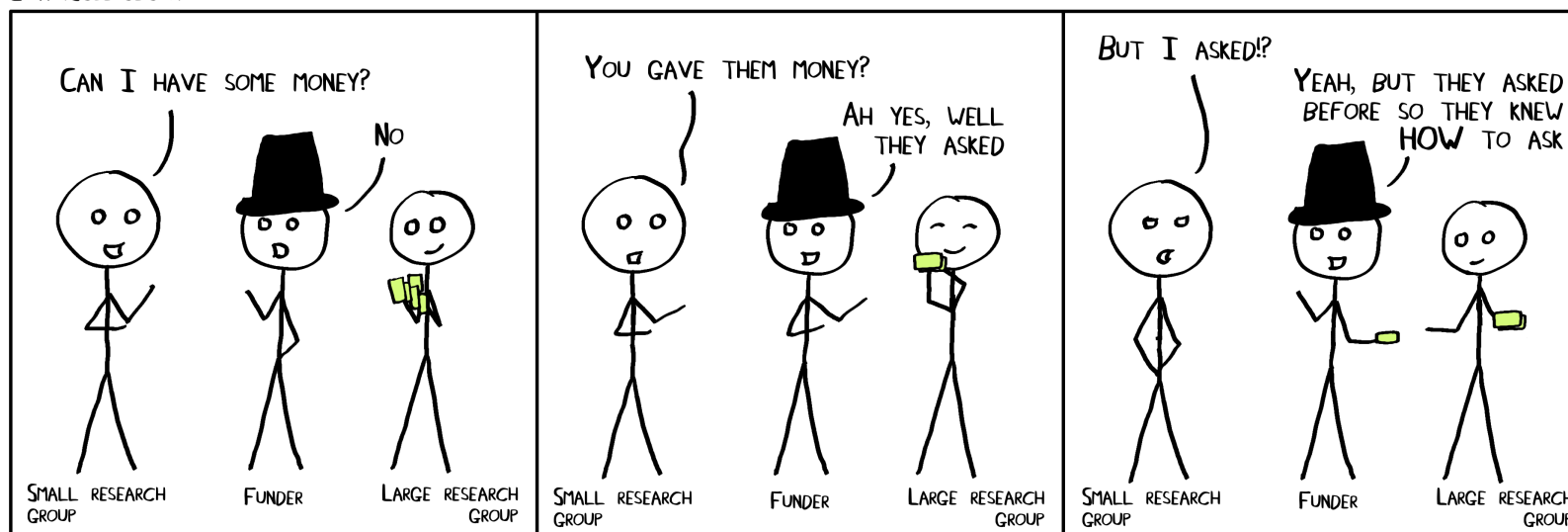
- ▶ Need suitable power sockets to charge / power electronic devices, or ways of charging devices away from power sources
- ▶ Need hardwired Internet or good quality WIFI for cloud-based software
- ▶ Will software need to be used offline e.g. on an archeological dig?
- ▶ Will hardware be at risk of contamination e.g. in a laboratory

# Financial Considerations

- ▶ **Licensing costs:** ELN Licenses, Custom Notetaking Licenses
- ▶ **Renovation costs:** Installing more power sockets/ethernet sockets / WIFI boosters
- ▶ **Power costs:** Facilitating charging of devices
- ▶ **Hardware costs:** Replacing legacy equipment, providing devices for digital capture (e.g. in the lab or in the field)
- ▶ **Maintenance & Development costs**
- ▶ **Staffing Costs:** Setup & Run ELN

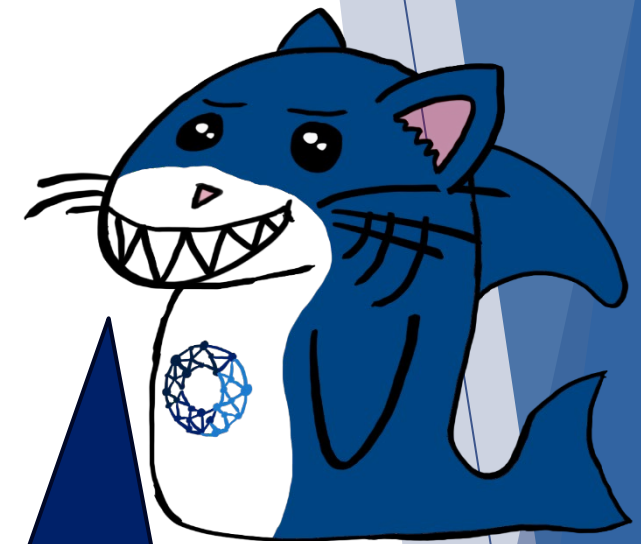
## UNIVERSITY FUNDING IN A NUTSHELL

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# Case Study Learnings

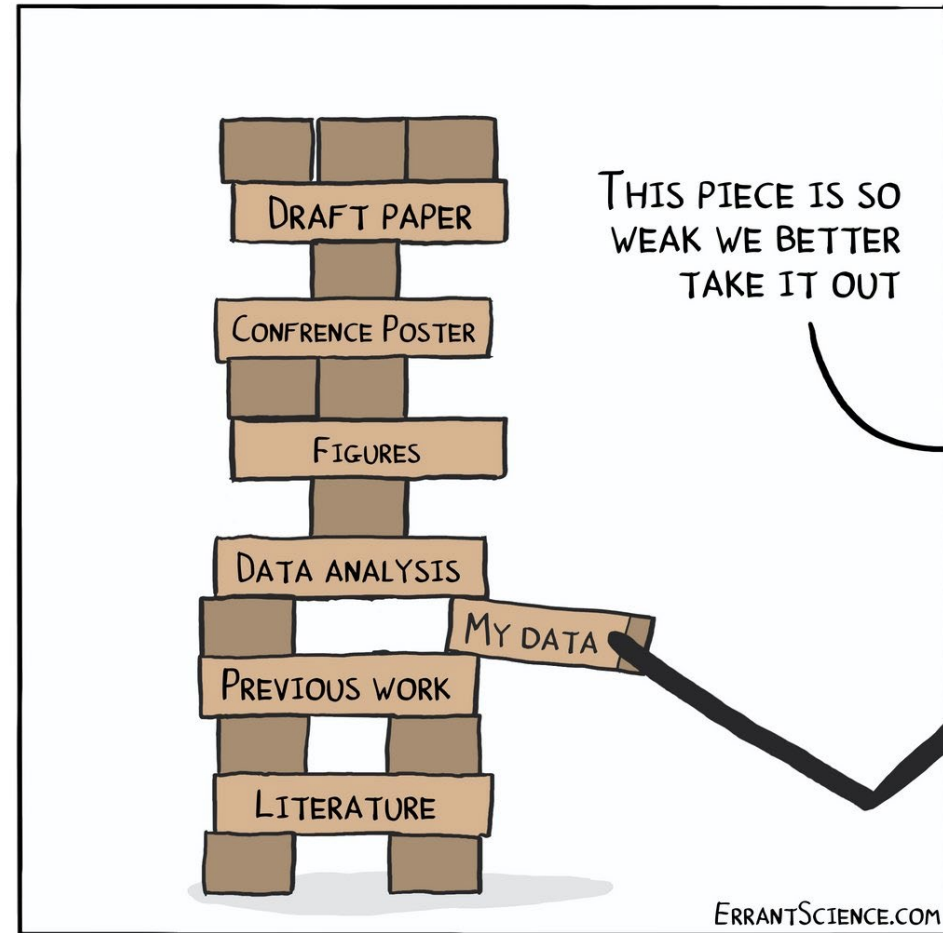
- ▶ One Note at Wellington
  - ▶ Implemented a policy where students starting in the first year needed to bring a MS Surface, existing students were given a choice, this permeated through to all students having surfaces after several years. Lab refurbed to have power sockets and space for devices.
- ▶ OneNote/AI4Green in Teaching labs at Nottingham
  - ▶ MS Surfaces purchased for the lab as part of refurb, Lab refurbed to have power sockets and space for devices.
- ▶ AI4Green in Postgraduate Lab
  - ▶ 1 Screen per fumehood raised above lab bench, tucked away mini PCs, mice and keyboard on benches, wired internet connection
- ▶ Revvity Signals
  - ▶ Group Leaders/Students asked about hardware preference, hardware obtained if desired



**DEDICATED LAB  
HARDWARE IS KEY!  
NO CROSS  
CONTAMINATION!**

# Data Considerations

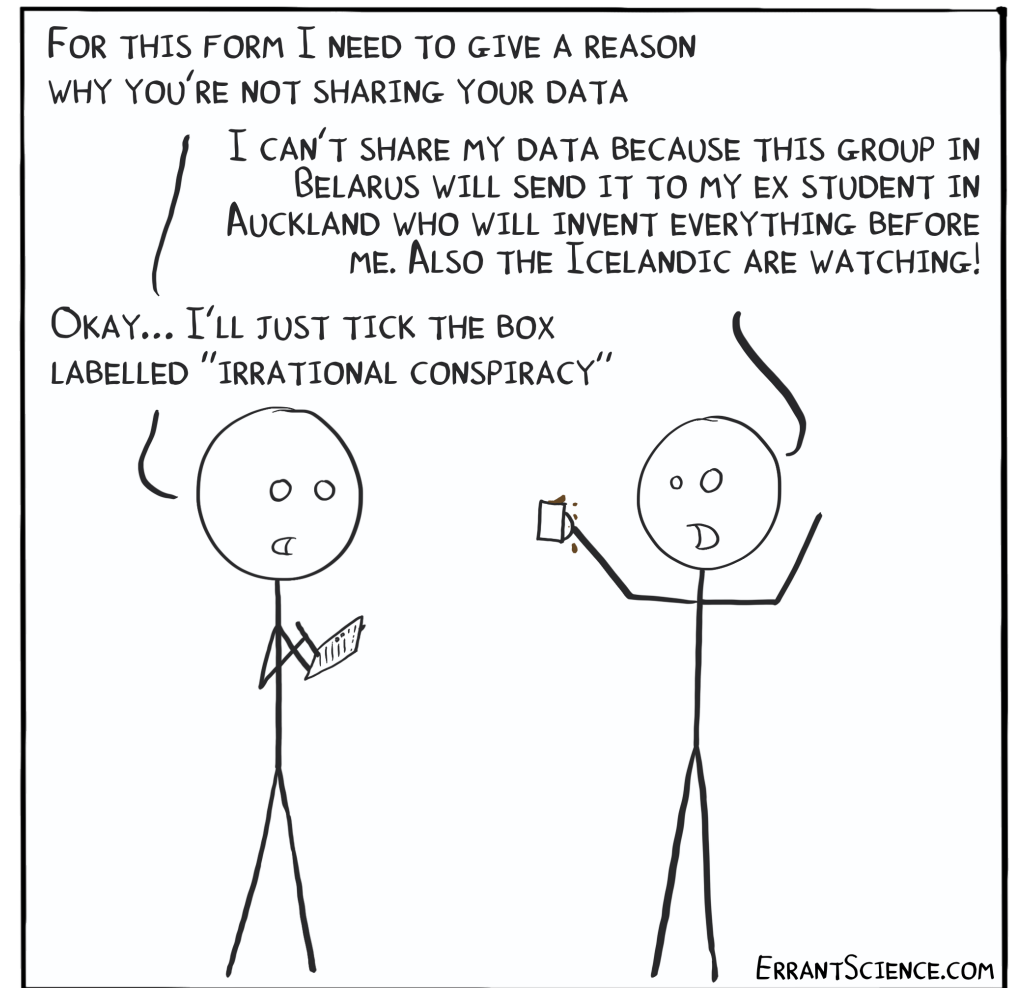
- ▶ Backup, Storage & Security
- ▶ Data Capture
- ▶ Experiment Templates
- ▶ FAIR Data
- ▶ Data Sharing
- ▶ Data Publishing





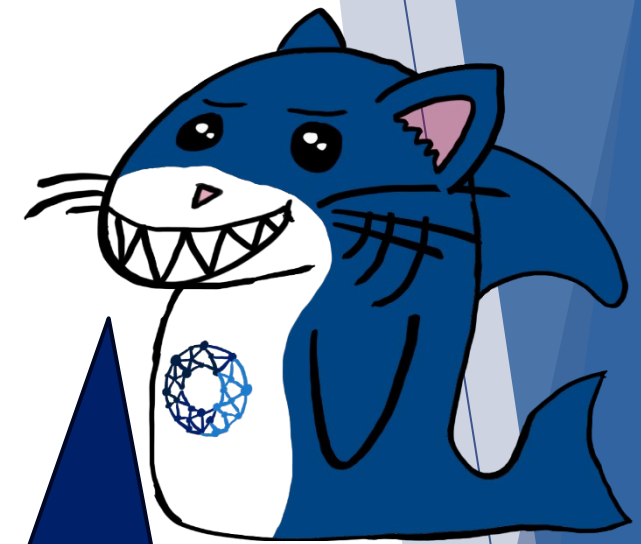
# Backup, Storage & Security

- ▶ Many researchers mistrust Digital Tools, particularly if they don't know where the data is stored
- ▶ There are concerns about data exit strategies – need to make sure data is stored and backed up in a way that this is feasible
- ▶ Consider what export functionalities are available?
- ▶ Security measures and vulnerabilities need to be considered



# Case Study Learnings

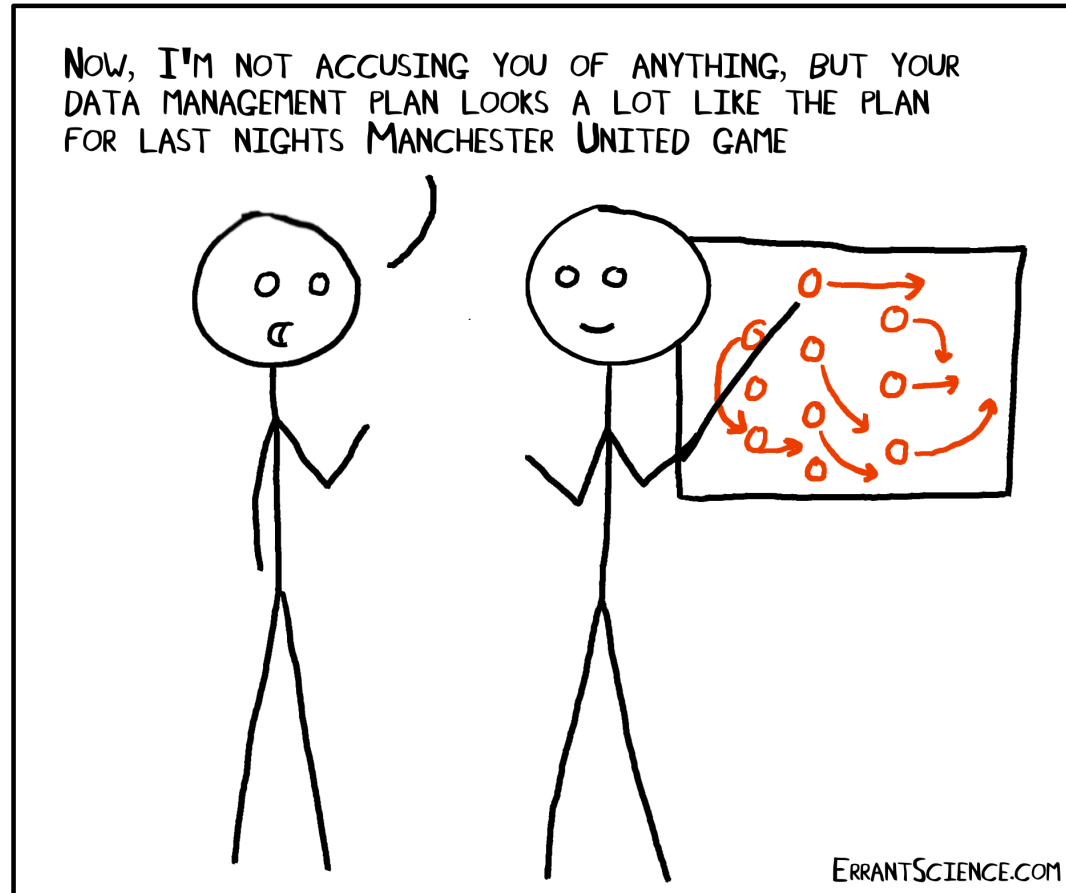
- ▶ Generic Notebook/OneNote
  - ▶ Backed up regularly as part of MS Ecosystem
- ▶ AI4Green
  - ▶ Custom made solution with embedded backups – less concern about vendor trust as this was an in-house solution
- ▶ Revvity Signals
  - ▶ Custom backup created pre trial using API, script runs daily to collect all closed experiments, providing a formal data exit strategy and additional backup in case of any issues



Trust & Data Exit Strategy is KEY! Always implement a Data Exit Strategy before putting your data into any new system!

# Data Capture / Templates

"QUALITY OF DATA MANAGEMENT  
PLANS REMAINS VARIABLE" #FIGSHAREFEST




[CC BY-ND 4.0](https://errantscience.com/) Errant Science - <https://errantscience.com/>

- ▶ Different domains will require different levels of data capture
- ▶ What data formats need to be supported for import/export?
- ▶ Consider the different types of data that will be recorded and make templates to ensure that all the relevant data is captured
- ▶ Fewer templates are ideal, but need to cover the range of data

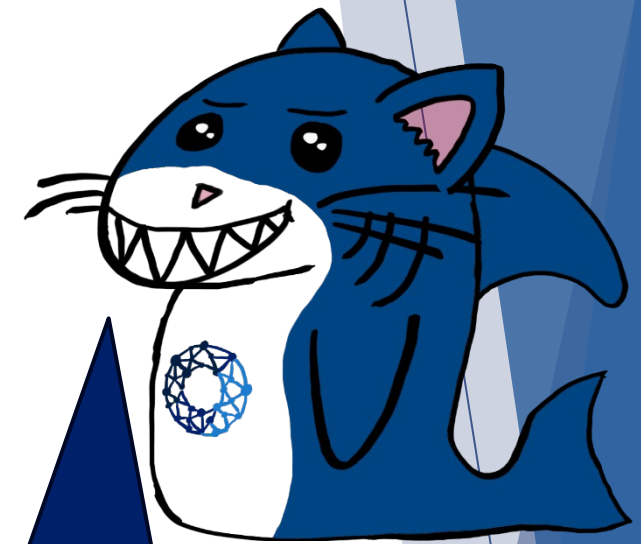
# Sharing / Publishing / FAIR Data

- ▶ A key reason to implement any Digital Notebook is to produce FAIRer Data for Publication – so your implementation plan needs to take this into account
- ▶ Another key reason is sharing data among colleagues/groups, its important to identify if people are finding it easier to locate relevant Digital Notebook entries to save time / inform

DATA PUBLISHING	
GOOD	BAD
DATA REPOSITORY	STICKY NOTE ON YOUR DOOR
INSTITUTIONAL ARCHIVE	SUPPLEMENTARY DATA
	BOTTOM OF A WELL
 ERRANTSCIENCE.COM	

Cartoon created by ErrantScience.com for AI4SD: licensed under [CC-BY-NC](https://creativecommons.org/licenses/by-nc/4.0/)

# Case Study Learnings



## ► Generic Notebook

- Simple Templates created to match lab and classroom work within the OneNote system.
- Notebooks shared between classes and teachers.

## ► AI4Green

- Structured sections for notes and writeup provided for students.
- Notebooks shared between classes and teachers (undergraduate labs) and between researchers and supervisors (postgraduate labs)

## ► Revvity Signals

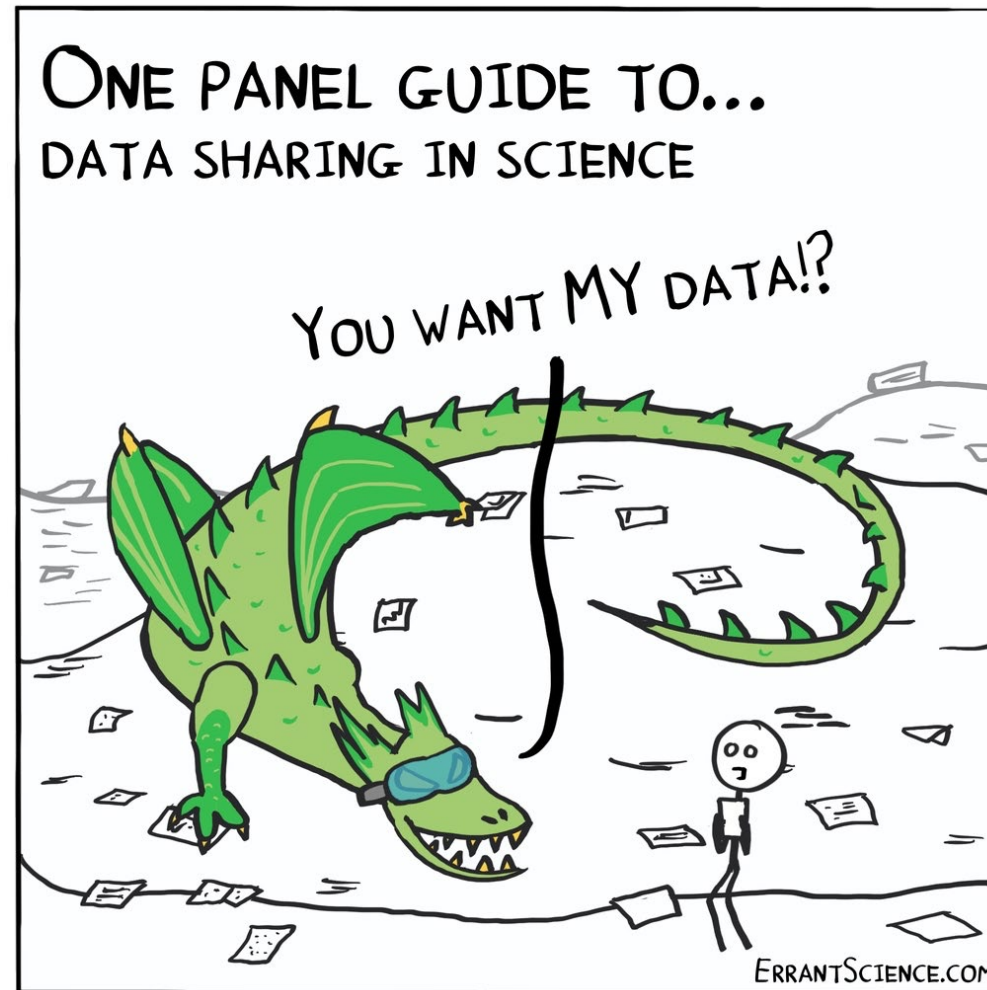
- Custom templates were created based on the areas of chemistry that the trial would be supporting
- Group Leaders dictated sharing across groups depending on privacy/embargo requirements. All notebooks shared with Group Leaders.

Work with the users and group leaders to create templates to capture structured relevant data!



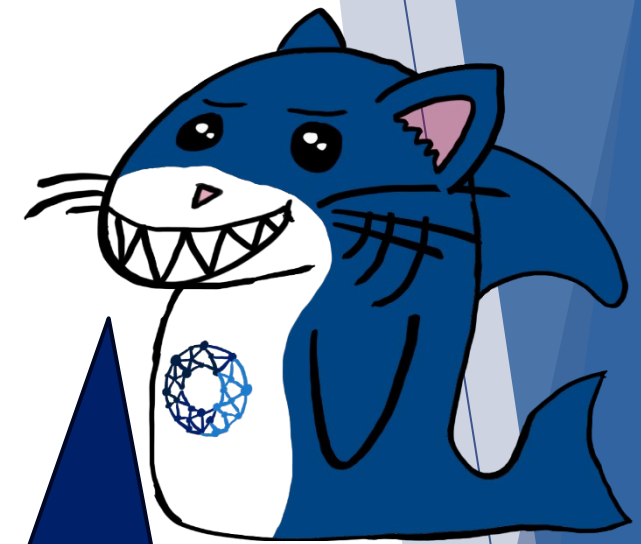
# Change Management / Adoption

- ▶ People are arguably one of the biggest barriers
- ▶ Top-down influence can make or break this
- ▶ Need to get the whole group on board
- ▶ Concerns about changing processes
- ▶ Hard to persuade people to embark on a journey with a lot of front-loaded work, unless they really understand the benefits



# Case Study Learnings

- ▶ Define the problem you are trying to solve
- ▶ Identify stakeholders, roles and required involvement
- ▶ Engage with relevant groups and hierarchies to fully understand the landscape
- ▶ Build a vision of success – make people understand the benefits and what you are trying to achieve



Regular Support IS  
KEY! Nobody will  
engage long term  
without it!

# How can PSDI Help?



Data Services



Data Tools



Community



Access to  
Data Sources



Guidance,  
Training &  
Case Studies



Collaboration

Find our resources on [www.psd.ac.uk](http://www.psd.ac.uk)!

# Knowledge Base

- ▶ The PSDI Knowledge Base will provide guidance for physical scientists, and those who support them, about a range of topics related to research data and PSDI technology and resources.



- ▶ A growing collection of content that can be built with the community.

# Software Selection – ELNFinder

<https://eln-finder.ulb.tu-darmstadt.de>

## ELN Finder

The ELN Finder helps you to search and select a suitable Electronic Lab Notebook (ELN) for your purposes.

- More than 40 filter criteria available.
- Filter criteria clearly divided into categories.
- Result list of the identified ELN tools displayed in an overview.
- Brief descriptions of the individual tools included.

 Find ELNs

**PSDI is proud to contribute to  
ELNFinder**

- ▶ Detailed hierarchical criteria catalogue created, defines and describes the metadata structure for the ELNs (Excel):
- ▶ > 40 criteria and associated values, attributes (e.g. name/URL).
- ▶ Summary of criteria in categories
- ▶ Fully functional first version developed on the basis of the open source software DSpace 7
- ▶ External ELN information collection created for individual ELNs
- ▶ Entering data from the information collection
- ▶ > 40 ELNs entered



# Data Revival Service

PSDI is providing a free version of the Data Revival Software

- ▶ This can be used to scan your handwritten lab book pages and turn them into machine-readable data
- ▶ Remember: Even if you implement digital notetaking tomorrow, there will still be a considerable amount of legacy data that may require digitisation



Scan in paper  
lab notebook  
pages

Convert into  
machine-  
readable  
content

Relational  
links across  
chemistry  
data

Semantic  
Search

High degree  
of accuracy

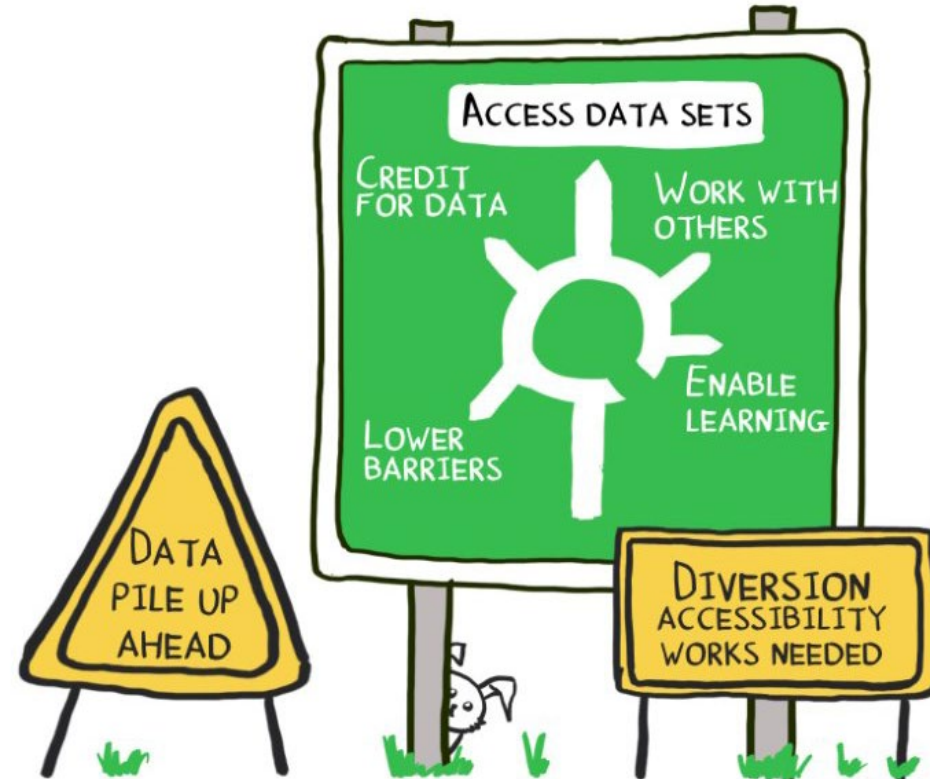
# Research Notebook Community



- ▶ PSDI are working to re-establish the Research Notebook Community
- ▶ Exploring anything and everything around Electronic Research Notebooks
- ▶ Many valuable case studies and resources!
- ▶ Aimed at all disciplines not just the sciences!
- ▶ **Mailing List**  
[RESEARCHNOTEBOOKS@jiscmail.ac.uk](mailto:RESEARCHNOTEBOOKS@jiscmail.ac.uk)
- ▶ **Website:**  
<https://researchnotebooks.wordpress.com/>  
(moving to [researchnotebooks.org](https://researchnotebooks.org))

# Conclusions

- ▶ This is a highly complex endeavour
- ▶ ALL of these considerations need to be taken into account – You need to ask the right questions
- ▶ You need to identify how to measure progress and success
- ▶ This requires dedicated time and people to make it happen
- ▶ PSDI are here to help!





# The Final Reveal



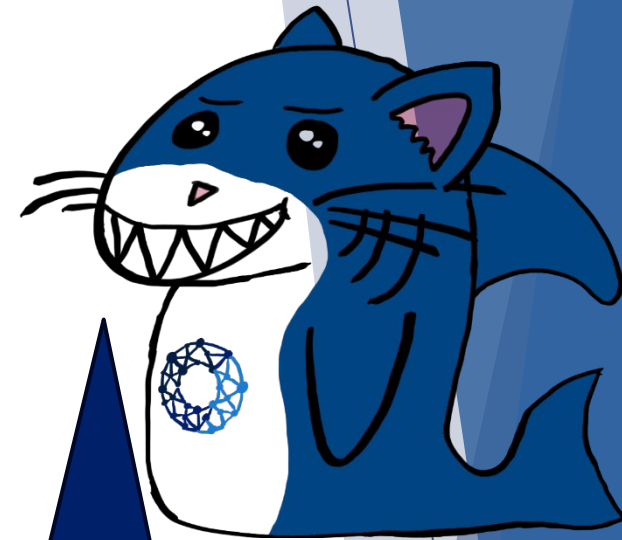
[https://www.reddit.com/r/MemeRestoration/comments/lynitm/agnes\\_winking\\_in\\_marvels\\_wandavision/](https://www.reddit.com/r/MemeRestoration/comments/lynitm/agnes_winking_in_marvels_wandavision/)  
<https://www.marvel.com/tv-shows/agatha-all-along/1>



It was Agatha all along! Hey who turned me into a witch?!

# Acknowledgements

- ▶ PhD Supervisory Team:
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- ▶ PSDI/Southampton ELN/OneNote Team:
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- ▶ ERN Community
  - ▶ Valerie McCutcheon, Cerys Willoughby
- ▶ AI4Green Team
  - ▶ Jonathan Hirst, Peace Nwafor, Cerys Willoughby, Katherine Jolley
- ▶ Wellington School
  - ▶ Caroline Evans, Jo Grundy
- ▶ Witchy Imagery
  - ▶ <https://collider.com/agatha-all-along-witch-references-end-credits/>



AND SHARKCAT!

If you want to see  
more of me sign up to  
our showcase!