PSDI

PHYSICAL SCIENCES
DATA INFRASTRUCTURE

Electronic Lab Notebooks and Beyond! The evolution of process recording tools for scientific research

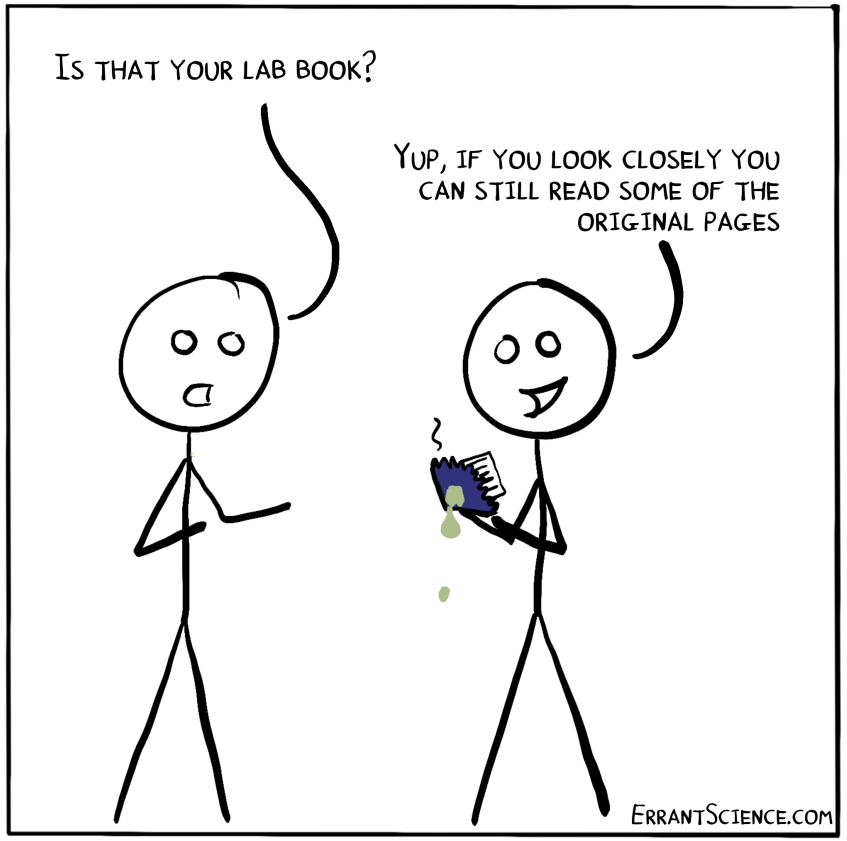
RSC Historical Group
13th March 2024
Dr Samantha Pearman-Kanza
University of Southampton

https://www.psdi.ac.uk/

PSDI
PHYSICAL SCIENCES
DATA INFRASTRUCTURE

Presentation Outline

- About Me
- Scientific Record Keeping & Electronic Lab Notebooks (ELNs)
- Barriers to ELNs
- The ELN Landscape and where ELNs fit into the wider Digital Landscape for Scientific Research
- Why does this matter? FAIR & Supplementary Information
- Examples of successful implementations
- Thoughts for the future
- PSDI Services & Research



PSDI
PHYSICAL SCIENCES
DATA INFRASTRUCTURE

About Me

- Senior Enterprise Fellow at University of Southampton
- Pathfinder Lead & Researcher for PSDI on Process Recording
- Researcher for AIChemy Hub on Process Recording
- Research Interests: Semantic Web Technologies, IoT, Research Data Management, Digitisation, Lab of the Future, Paperless Labs, Re-use of Technology
- @SamiKanza

PSDI
PHYSICAL SCIENCES
DATA INFRASTRUCTURE

How did I end up here?

BMC Part of Springer Nature Search Menu

Journal of Cheminformatics

Home About Articles Submission Guidelines About The Editors Calls For Papers

Download PDF

Research article | Open Access | Published: 24 May 2017

Electronic lab notebooks: can they replace paper?

Samantha Kanza, Cerys Willoughby, Nicholas Gibbins, Richard Whitby, Jeremy Graham Frey, Jana Erjavec, Klemen Zupančič, Matjaž Hren & Katarina Kovač

Journal of Cheminformatics **9**, Article number: 31 (2017) | Cite this article

14k Accesses | **20** Citations | **78** Altmetric | Metrics

Abstract

Despite the increasingly digital nature of society there are some areas of research that remain firmly rooted in the past; in this case the laboratory notebook, the last remaining paper component of an experiment. Countless electronic laboratory notebooks (ELNs) have been created in an attempt to digitise record keeping processes in the lab, but none of them have become a 'key player' in the ELN market, due to the many adoption barriers that have been identified in previous research and further explored in the user studies presented here. The main issues identified are the cost of the current available ELNs, their ease of use (or lack of it) and their accessibility issues across different devices and operating systems. Evidence suggests that whilst scientists willingly make use of generic notebooking software, spreadsheets and other general office and scientific tools to aid their work, current ELNs are lacking in the required functionality to meet the needs of the researchers. In this paper we present our

nature

View all journals Search Login

Explore content About the journal Publish with us Subscribe Sign up for alerts RSS feed

nature > toolbox > article

TOOLBOX | 06 August 2018

How to pick an electronic laboratory notebook

Choosing wisely from a burgeoning array of digital tools can help researchers to record experiments with ease.

Roberta Kwok

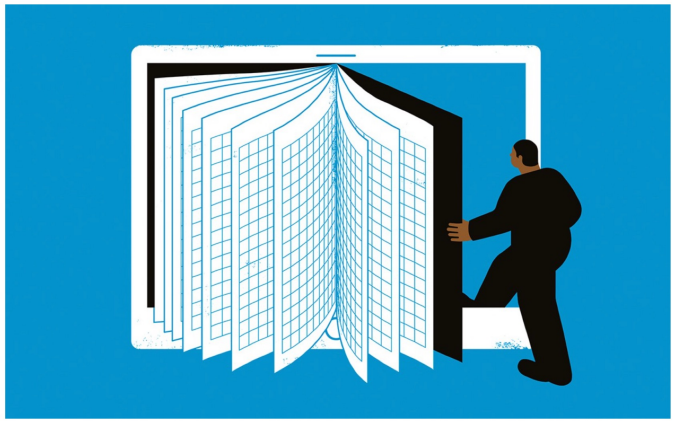


Illustration by The Project Twins

Since at least the 1990s, articles on technology have predicted the imminent, widespread adoption of electronic laboratory notebooks (ELNs) by researchers. It has yet to happen – but more and more scientists are taking the plunge.

One barrier to uptake is the wide range of products available. ELNs comprise software that helps researchers to document experiments, and that often has features such as protocol templates, collaboration tools, support for electronic signatures and the ability to manage the lab inventory. But the ELN market encompasses considerable variety; a study conducted in 2016 by the University of Southampton, UK, identified 72 active products (S. Kanza *et al. J. Cheminformatics* **9**, 31; 2017). "It's just insane," says Sian Jones, a petroleum engineer at the Delft University of Technology in the Netherlands. "It does become very confusing." And many researchers simply lack the time or motivation to make the move to ELNs.

Access this article via **University of Southampton**

Download PDF

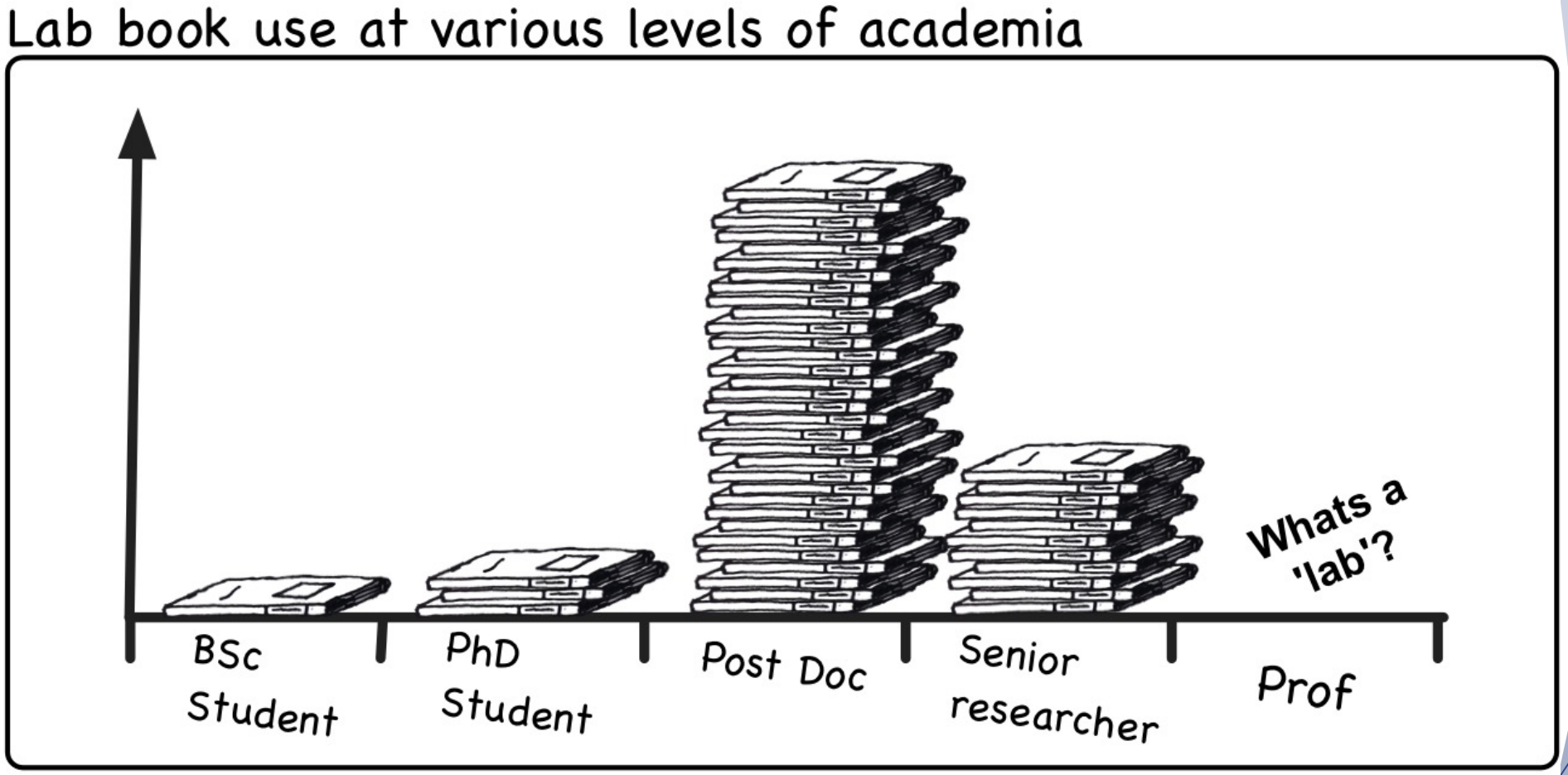
Subjects

Lab life Research management Research data Technology

Personal Photograph of Dr Samantha Pearman-Kanza

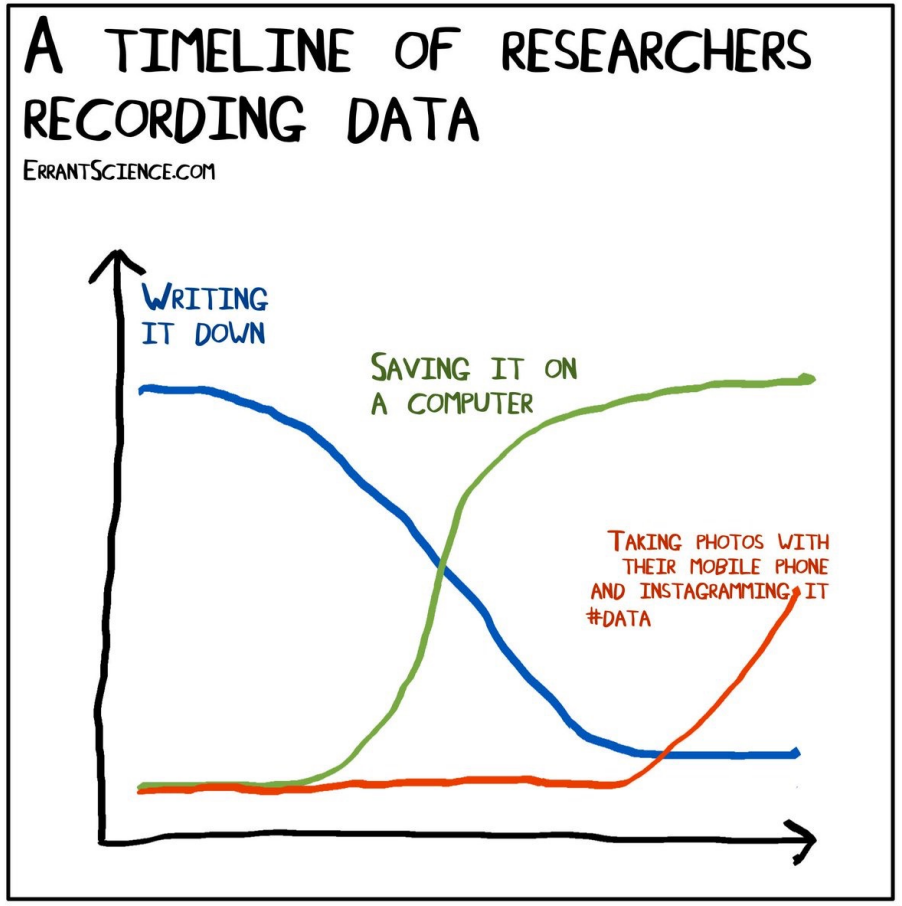
PSDI
PHYSICAL SCIENCES
DATA INFRASTRUCTURE

Scientific Record Keeping & Electronic Lab Notebooks (ELNs)



PSDI
PHYSICAL SCIENCES
DATA INFRASTRUCTURE

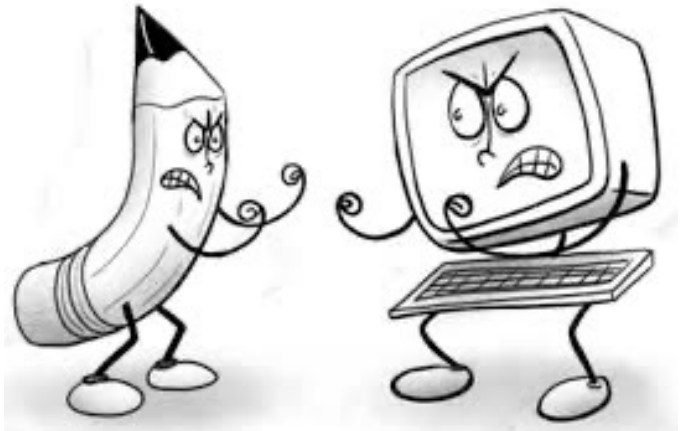
Scientific Record Keeping



- Scientists keep records of their work.
- Typically using a paper lab notebook.
- This tradition that still holds strong in many labs today!

PSDI
PHYSICAL SCIENCES
DATA INFRASTRUCTURE

Paper vs Electronic



"It Was A Normal Day Of Office When A Sweet Voice Break - Computer Vs Paper" – free download from SeekPNG

Advantages

- Cheap
- Portable
- Robust
- Can be securely stored
- Ease/Flexibility of Data Entry
- Doesn't require a power supply (or access to power)

Disadvantages

- Easy to lose/destroy
- Harder to search
- Harder to backup
- Harder to share
- Frequently gets forgotten
- Harder to readily access from multiple locations

PSDI
PHYSICAL SCIENCES
DATA INFRASTRUCTURE

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

PSDI
PHYSICAL SCIENCES
DATA INFRASTRUCTURE

The Electronic Lab Notebook

- ELNs were originally created to serve as a direct replacement for the paper lab notebook…..Which sounds like a simple endeavour at first….!

"Electronic Lab Notebooks are great, but not on vacation" Cartoon by Phil Johnson for MIT.

Advantages

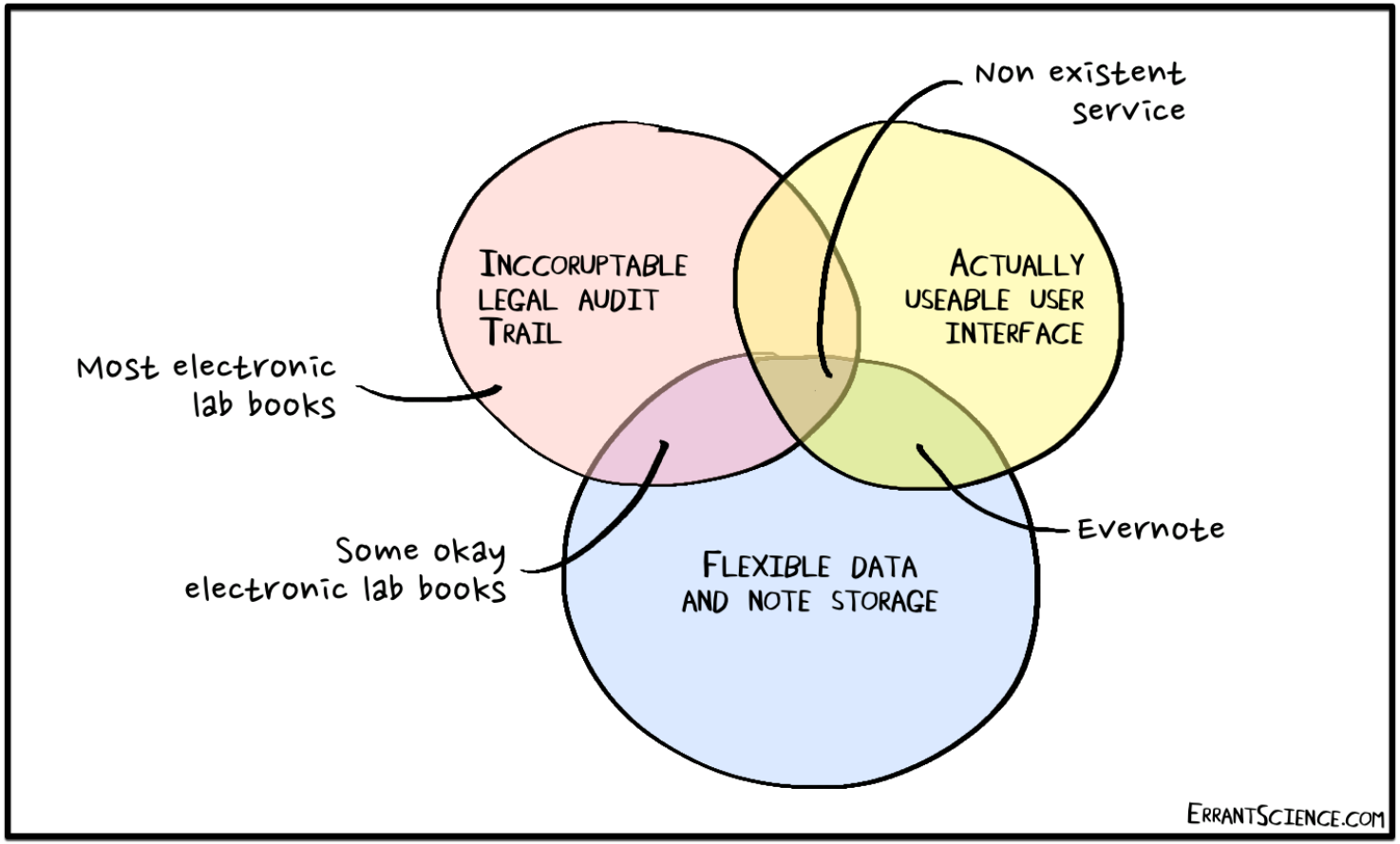
- Accessible from multiple locations
- Searchable
- Easy to backup
- Easy to share data
- Data is quickly retrievable
- Can be used by multiple people at once

Disadvantages

- Expensive potentially
- Slower/inflexible data entry
- Requires power supply/power
- May require internet
- Concerns about tech in labs
- Harder to create diagrams

PSDI
PHYSICAL SCIENCES
DATA INFRASTRUCTURE

Barriers to ELNs



A venn diagram guide to electronic lab books

PSDI
PHYSICAL SCIENCES
DATA INFRASTRUCTURE

Choice Barriers

There are now over 80 active ELNs on the market!

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

PSDI
PHYSICAL SCIENCES
DATA INFRASTRUCTURE

Requirements Barriers

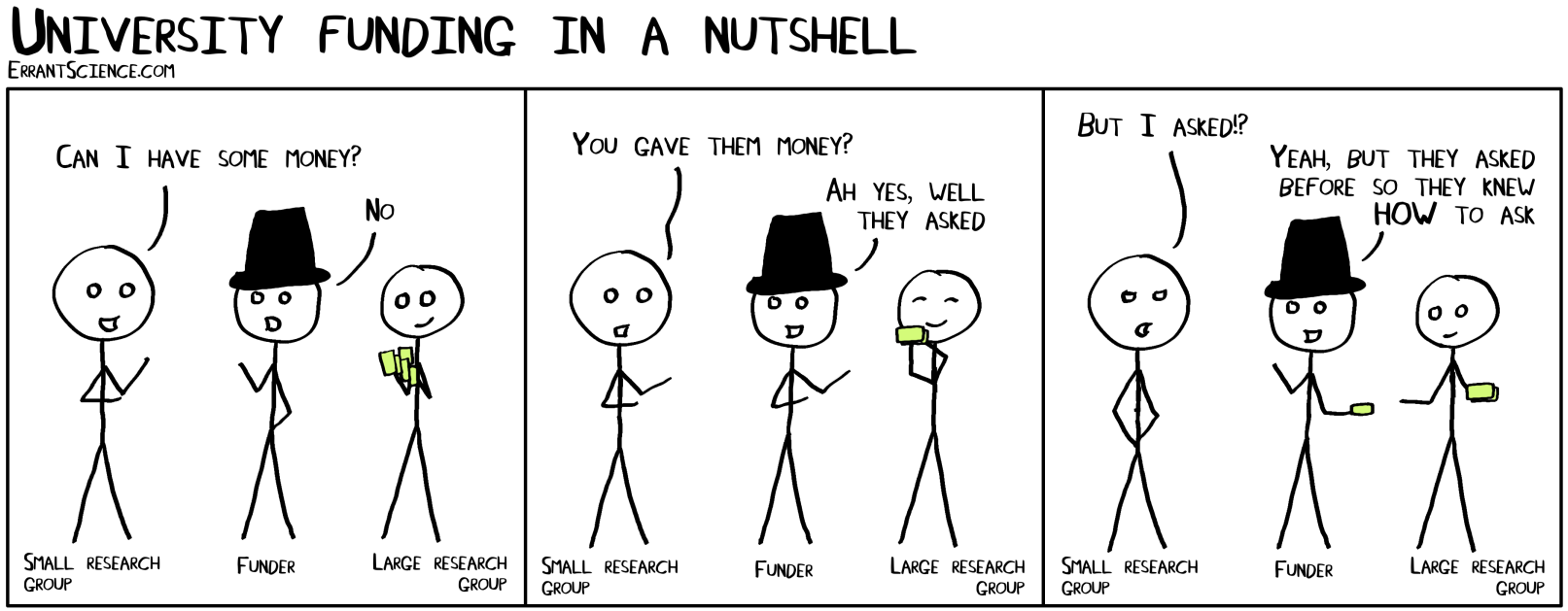
- There is no one “ELN to rule them all”
- How can you expect an ELN to cater to the diverse needs of an entire university, across the whole range of scientific disciplines and stages of education?
- What works for one group/lab almost certainly work for another

Diagram from 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

PSDI
PHYSICAL SCIENCES
DATA INFRASTRUCTURE

Cost Barriers

- ELN Licensing costs
- Hardware costs - Replacing legacy equipment, Providing devices to use ELN on
- Lab renovation costs - Installing more power sockets/ethernet sockets / WIFI boosters
- Maintenance costs
- Potential future development costs



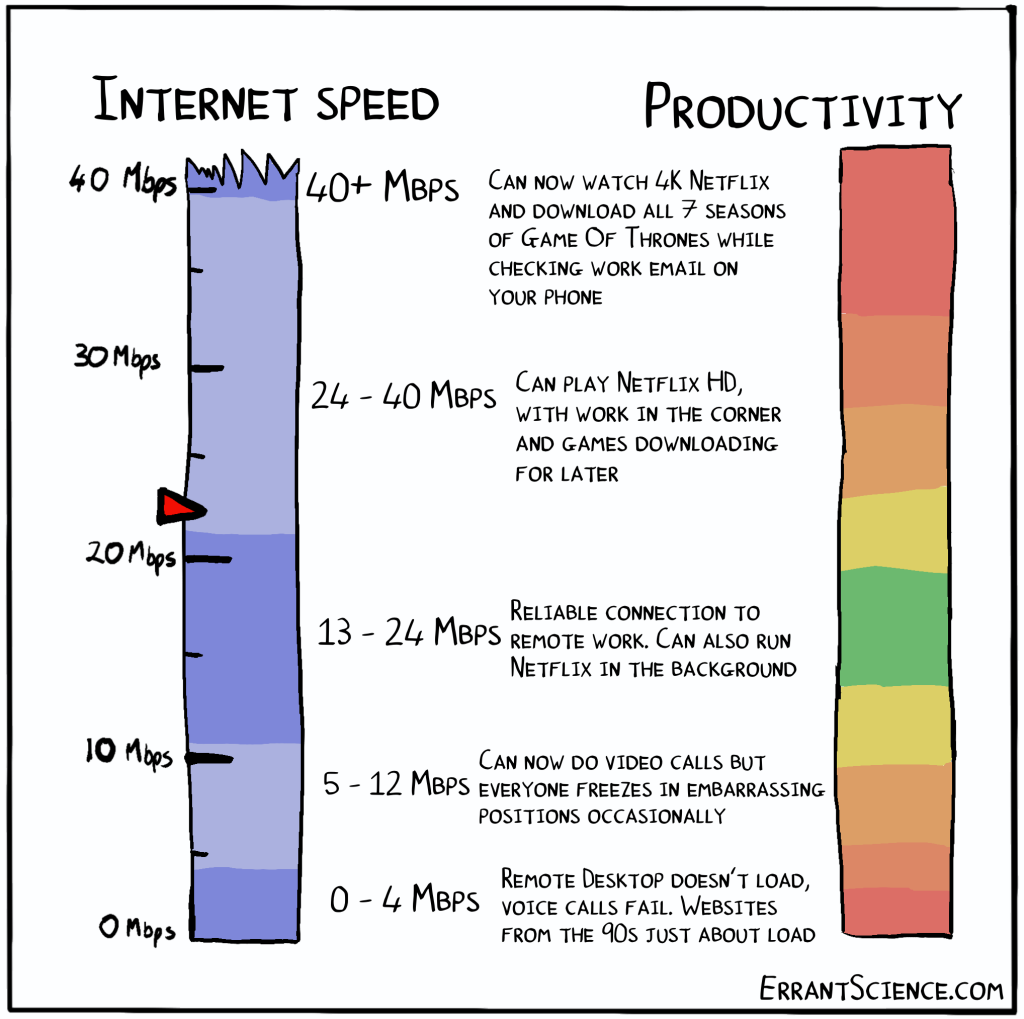
PSDI
PHYSICAL SCIENCES
DATA INFRASTRUCTURE

Time Barriers

- You can't implement any new system overnight
- You need to consider
  - Implementation time
  - Training time
  - How moving systems may impact researchers and how that can be accounted for
  - Potential duplication of data entry depending on setup

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

Hardware Barriers



Hardware Devices

- What electronic devices are going to be used?
- Space to use/store electronic devices
- Internet/WIFI connection required

Hostile Environment for Hardware

- Chemical spills on keyboards/computers
- Magnetised equipment that destroys electronic devices
- Cross contamination moving devices in and out of the lab

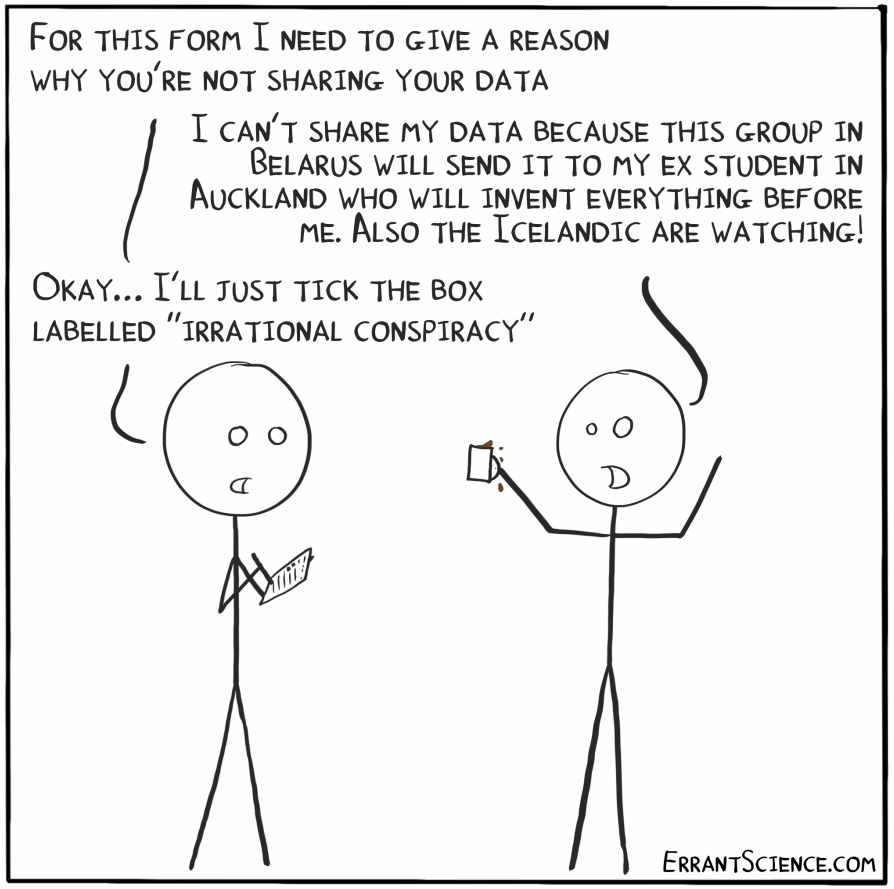
Compatibility Concerns

- Will an ELN be interoperable with legacy hardware equipment?

PSDI
PHYSICAL SCIENCES
DATA INFRASTRUCTURE

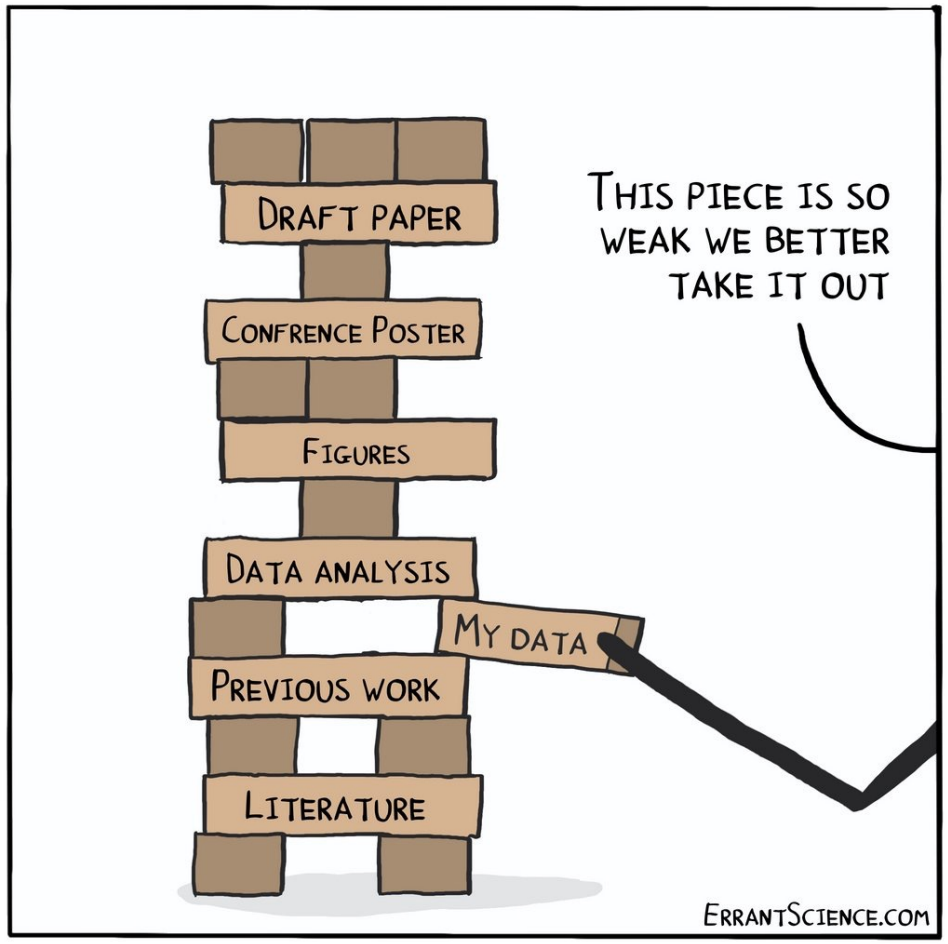
Trust Barriers

- Many researchers do not trust ELNs
- There are many concerns to consider:
  - Data privacy (Sharing/Hacking)
  - ELNs using proprietary formats
  - Lack of cohesive data exit strategy



PSDI
PHYSICAL SCIENCES
DATA INFRASTRUCTURE

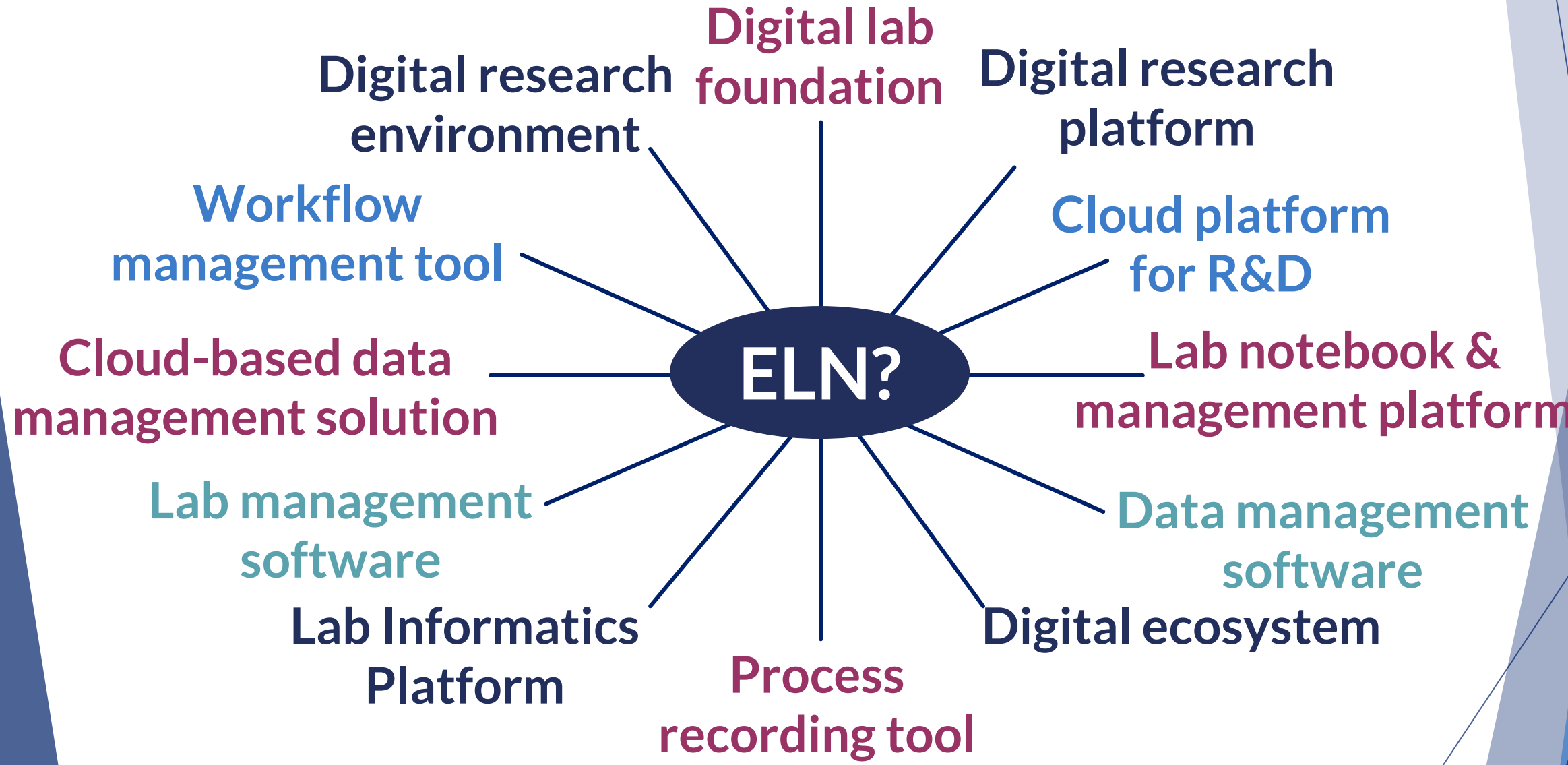
People/Adoption Barriers



- 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

PSDI
PHYSICAL SCIENCES DATA INFRASTRUCTURE

The ELN Landscape and where ELNs fit into the wider Digital Landscape for Scientific Research

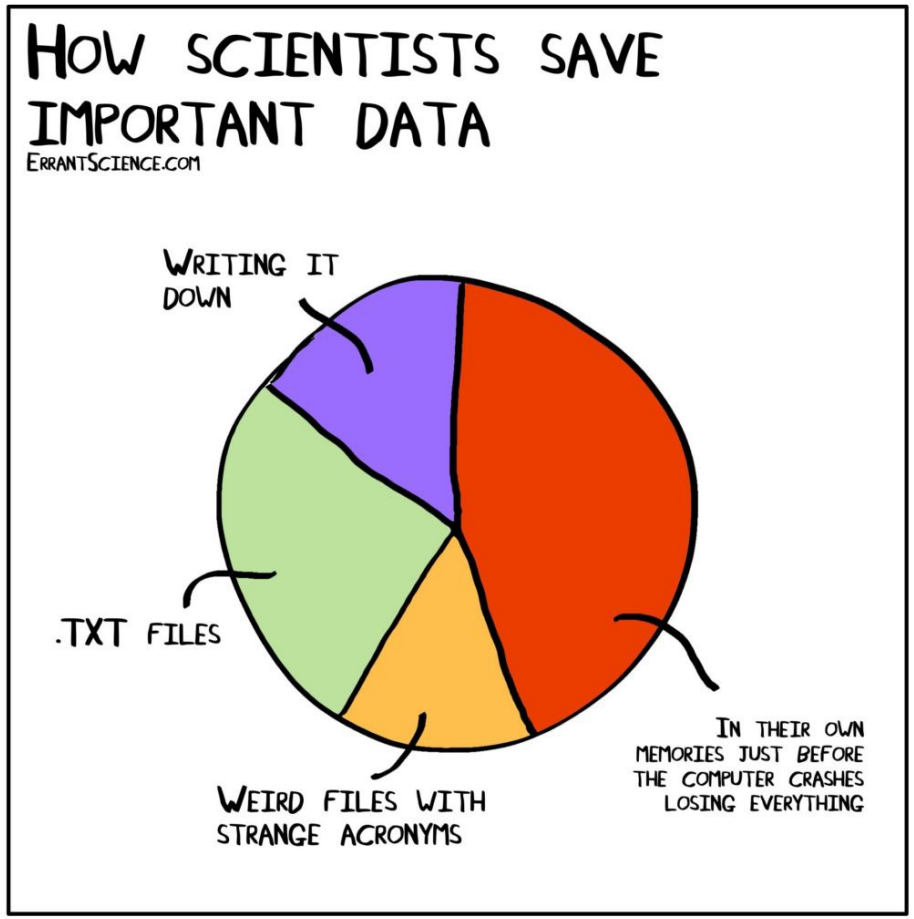


PSDI
PHYSICAL SCIENCES
DATA INFRASTRUCTURE

Evolution of Tools

- Frequently these platforms encompass one of many of:
  - ELNs (Electronic Lab Notebooks)
  - LIMS (Laboratory Information Management System)
  - SDMS (Scientific Data Management System)
  - Inventory / Sample Management
  - Registry

They are no longer
JUST A REPLACEMENT



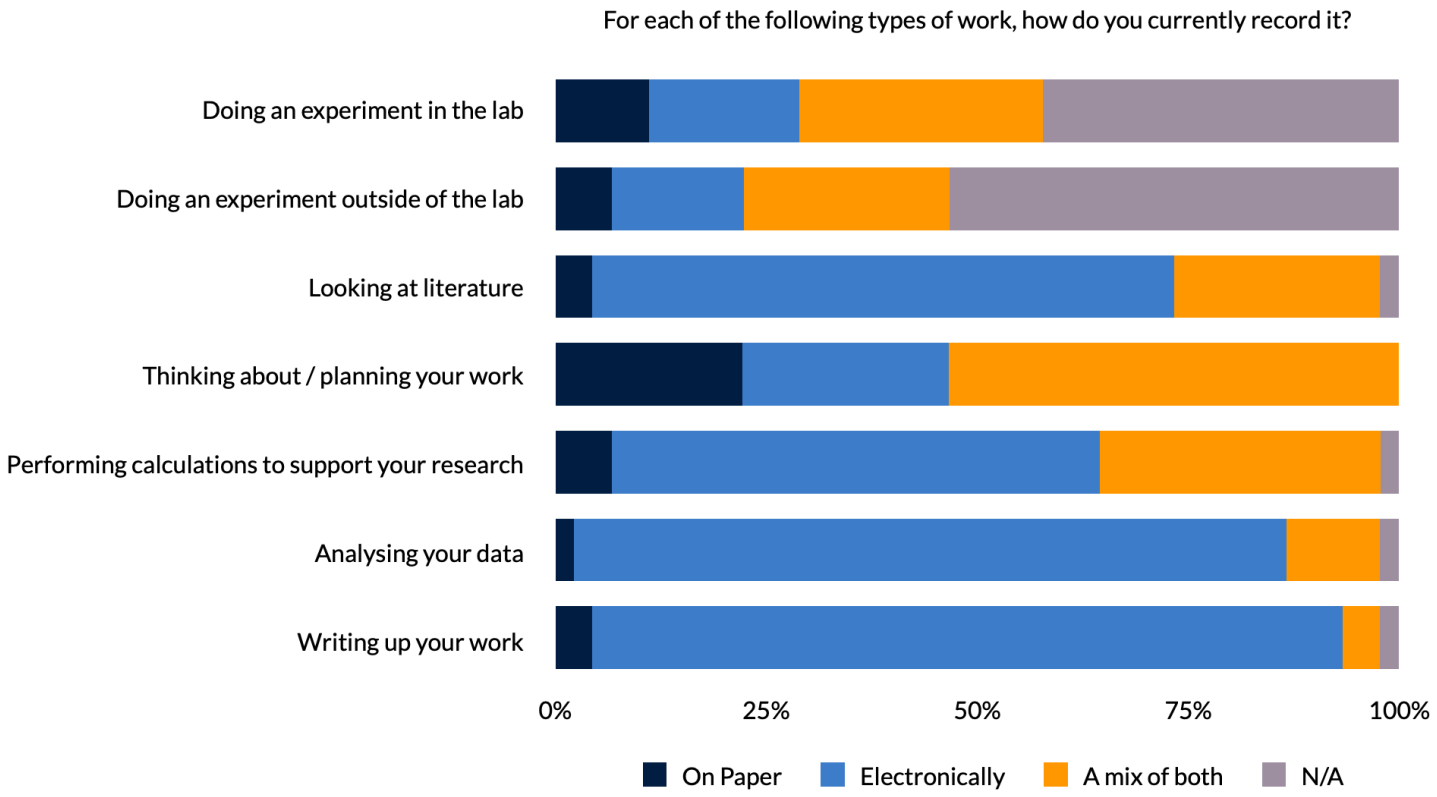
PSDI
PHYSICAL SCIENCES
DATA INFRASTRUCTURE

Research & Surveying our community

- Two surveys
  - Digital Requirements Survey
  - Process Recording Survey
- Extensive ELN Market Research
  - Discussions with Vendors
  - Discussions with Universities

PSDI
PHYSICAL SCIENCES
DATA INFRASTRUCTURE

Use of Paper & Electronic

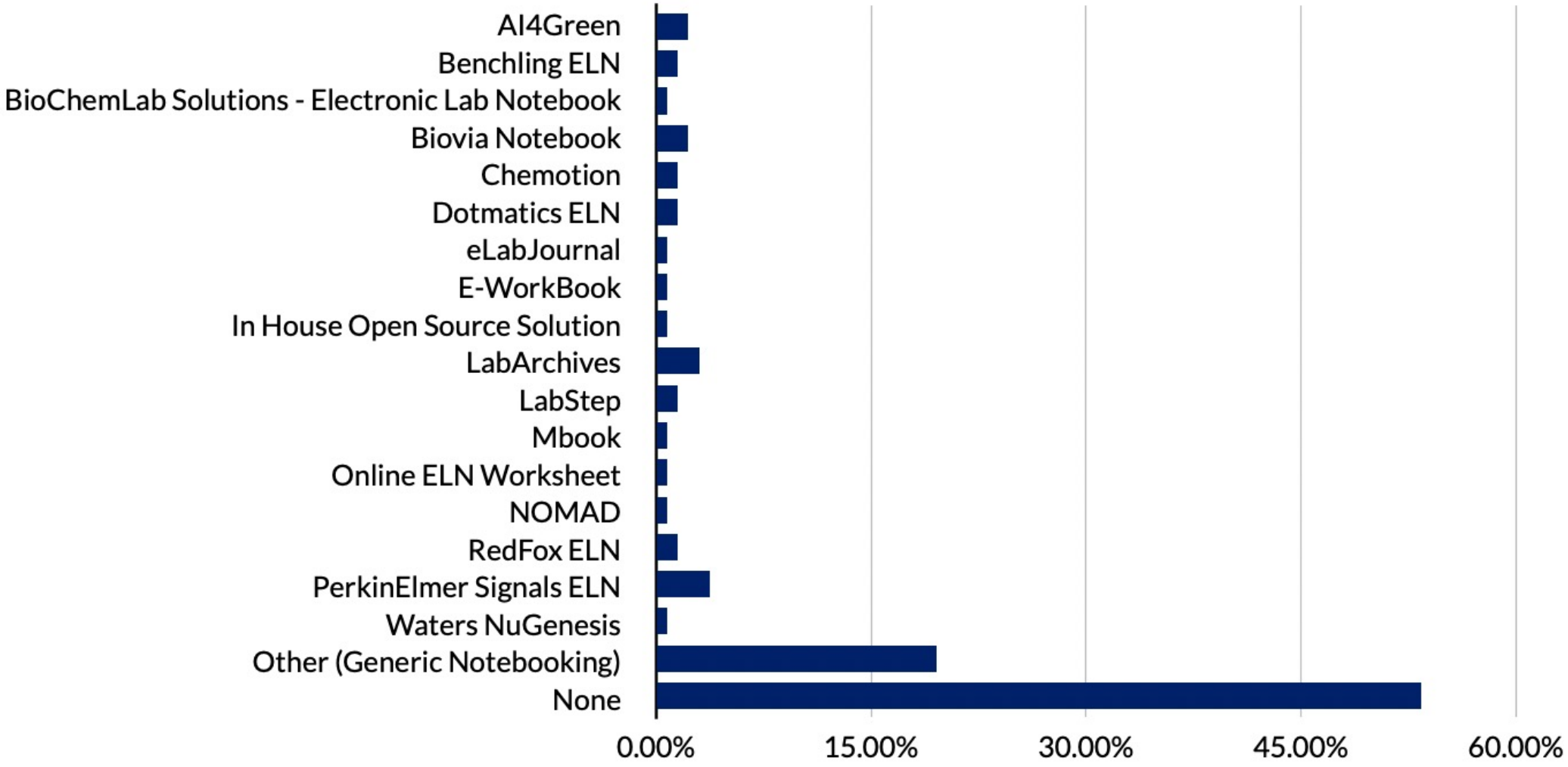


Researchers work in different ways using a mix of paper/electronic methods

Paper is used more for planning, with a heavy reliance on digital methods for analysis and writeup

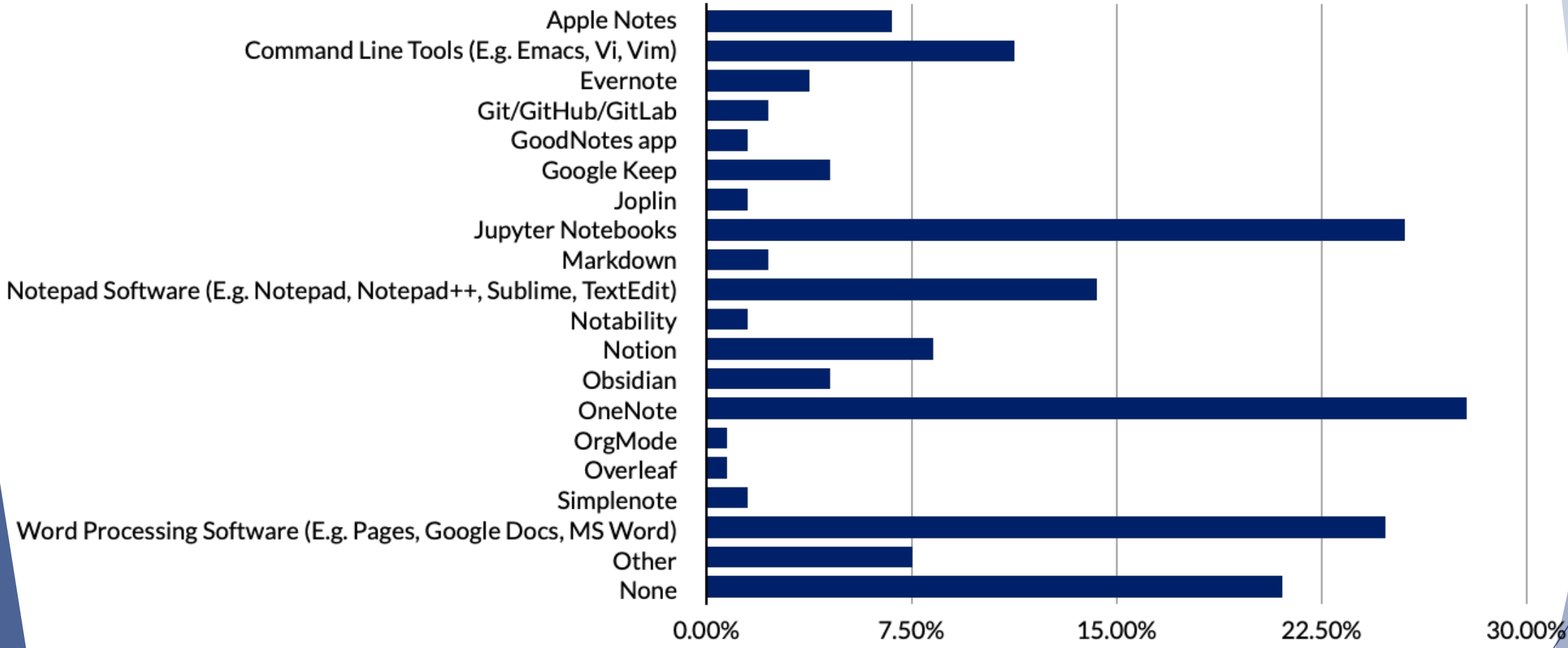
PSDI
PHYSICAL SCIENCES
DATA INFRASTRUCTURE

What ELNs do you use?



PSDI
PHYSICAL SCIENCES
DATA INFRASTRUCTURE

What Generic Notebooking Tools do you use?



PSDI
PHYSICAL SCIENCES
DATA INFRASTRUCTURE

What other software do you use?

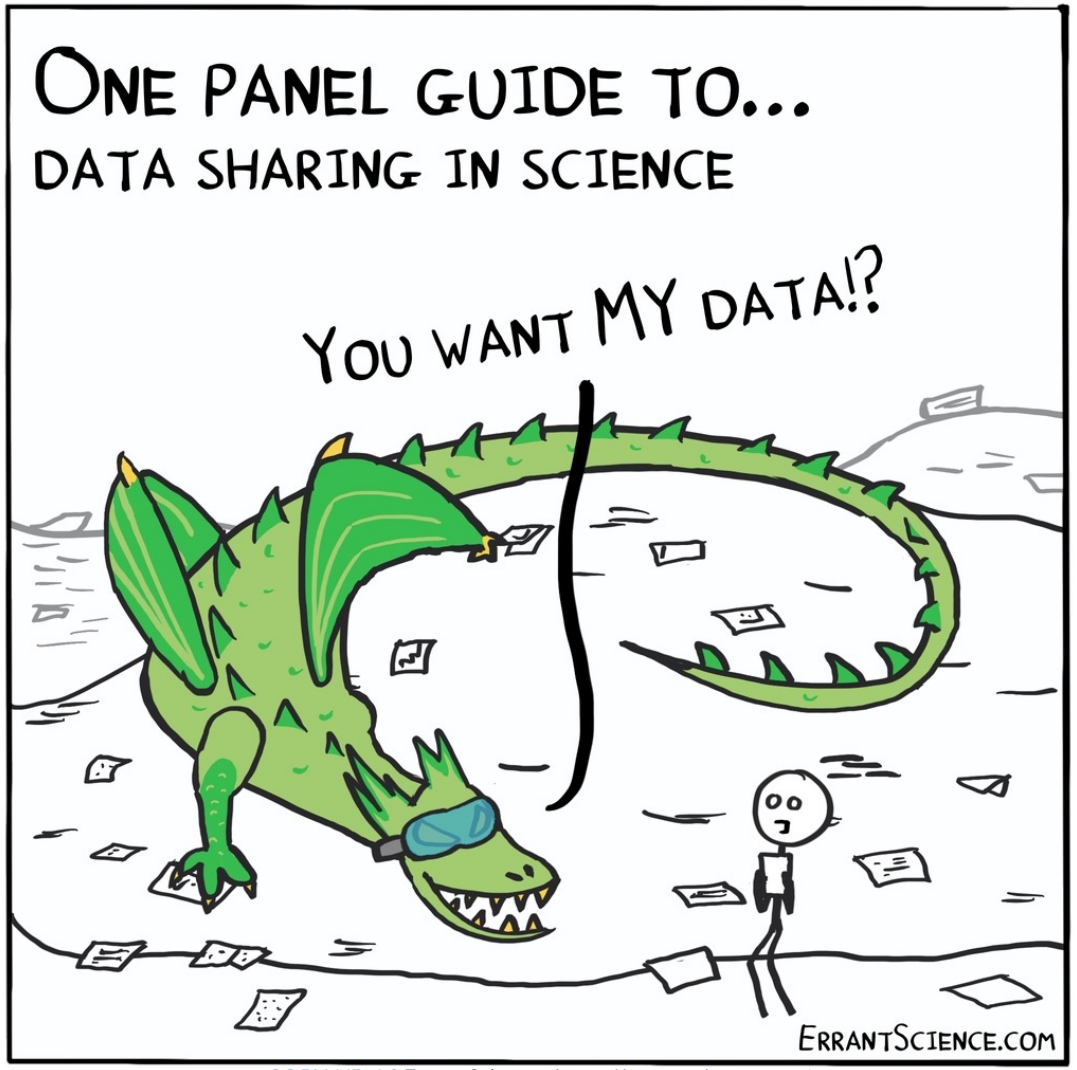
Category	Totals (/206)	Percentage
Crystallographic Software	26	12.44%
Coding Software	22	10.53%
Molecular Modelling & Simulation Software	22	10.53%
Quantum Chemistry and Solid State Physics Software	21	10.05%
Data Visualisation & Analysis	19	9.09%
General document processing	18	8.61%
Other	13	6.22%
Spectroscopic Software	10	4.78%
Image processing Software	9	4.31%
Chemical Database & Informatics Software	8	3.83%
Organisational Software	7	3.35%
Chemistry Bibliographic Databases	5	2.39%
Database Software	5	2.39%
Instrument Control	5	2.39%
Simulation (non-chemical)	5	2.39%
Communication Software	4	1.91%
Molecular Editor Software	3	1.44%
Nanostructures Modelling Software	2	0.96%
Machine Learning	2	0.96%
CAD Software	2	0.96%
Workflow software	1	0.48%

What other software do you use in your work?

- >200 different software packages identified
- Categorised using categories from PhD research and identified additional categories
- Demonstrates the wide ranging need for generic and specialist software in the physical sciences

PSDI
PHYSICAL SCIENCES
DATA INFRASTRUCTURE

Why does this matter? FAIR & Supplementary Information



PSDI
PHYSICAL SCIENCES
DATA INFRASTRUCTURE

What is this all for?

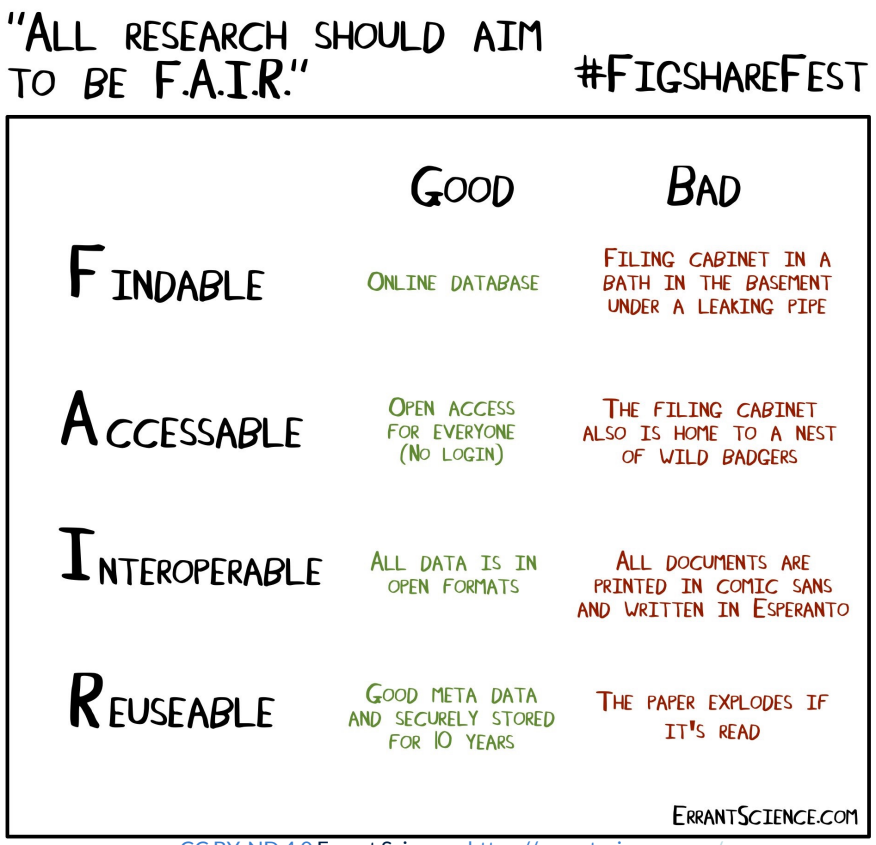
- We should be recording our data and methods for:
  - Our future selves to access
  - To share with the wider scientific community and to add to the greater body of knowledge
  - To make our data/methods FAIR

PSDI
PHYSICAL SCIENCES
DATA INFRASTRUCTURE

What does FAIR mean?

From 'The FAIR Guiding Principles for scientific data management and stewardship'[1]

- F – Findable
- A – Accessible
- I – Interoperable
- R – Reusable

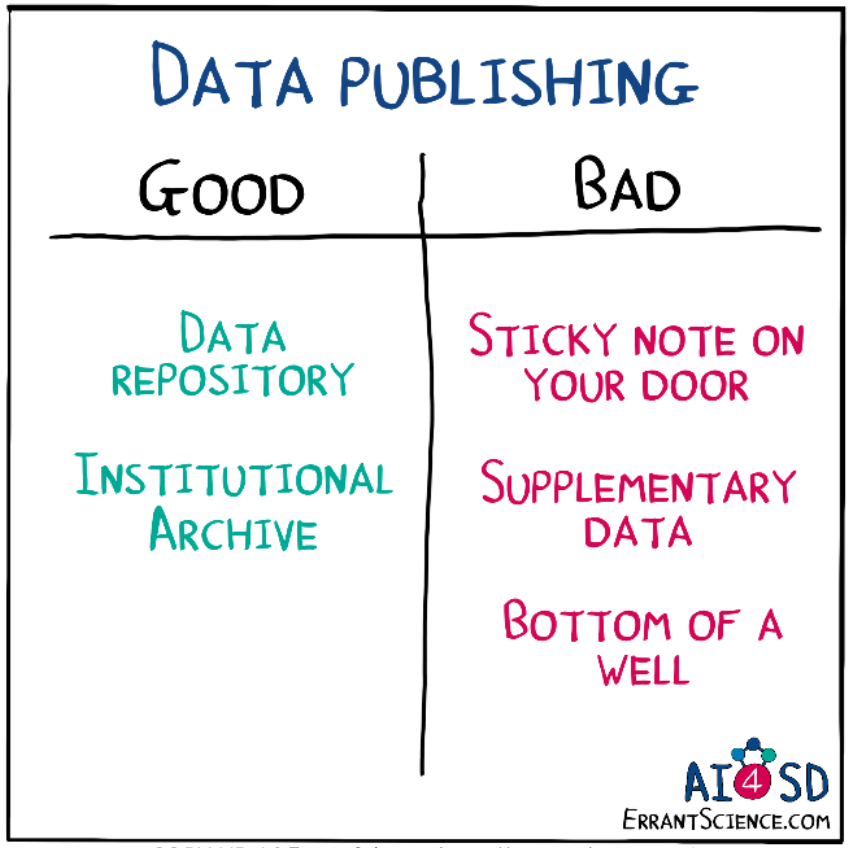


[1] Wilkinson, M., Dumontier, M., Aalbersberg, I. *et al.* The FAIR Guiding Principles for scientific data management and stewardship. *Sci Data* **3**, 160018 (2016). https://doi.org/10.1038/sdata.2016.18

PSDI
PHYSICAL SCIENCES
DATA INFRASTRUCTURE

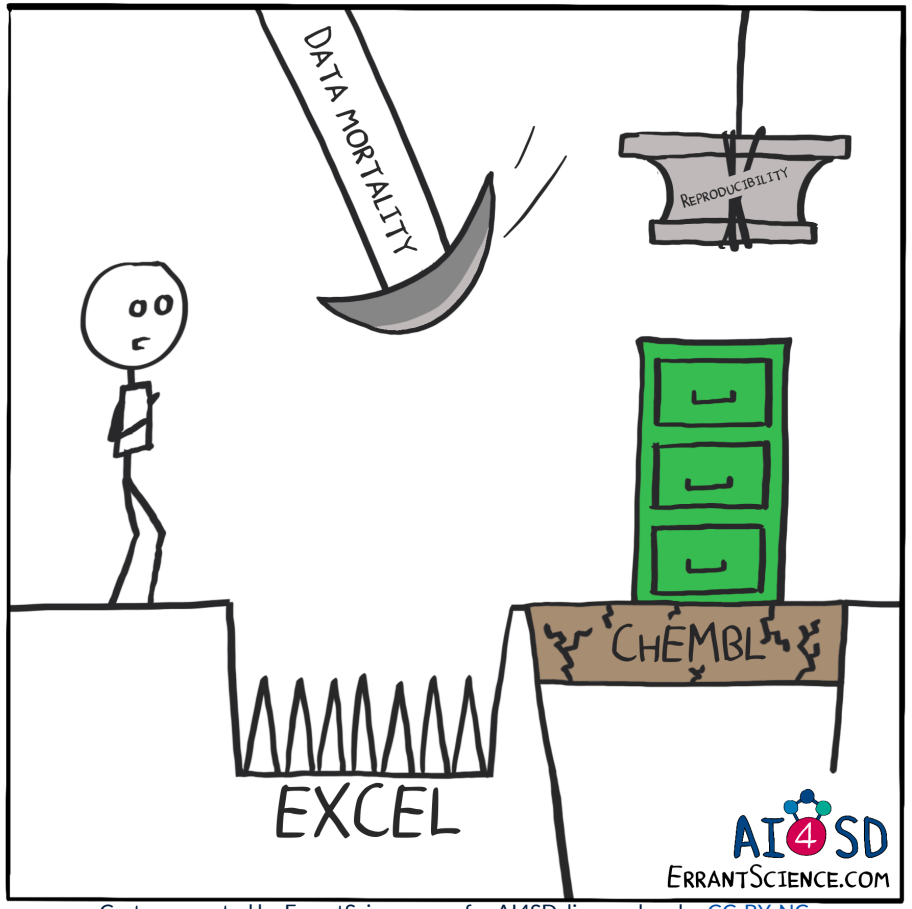
FAIR Considerations

- This isn't JUST about the data
- You need to consider:
  - Data, Tools, Code, Methods, Context
  - How could/would your work be re-used, replicated, reproduced or repurposed
    - Re-use – re-use the data (or run the software) in the same manner
    - Replicate – repeat entire research from scratch including data collection and analysis
    - Reproduce – reanalyse the existing data in the same manner
    - Repurpose – use existing data or software for a new purpose



PSDI
PHYSICAL SCIENCES
DATA INFRASTRUCTURE

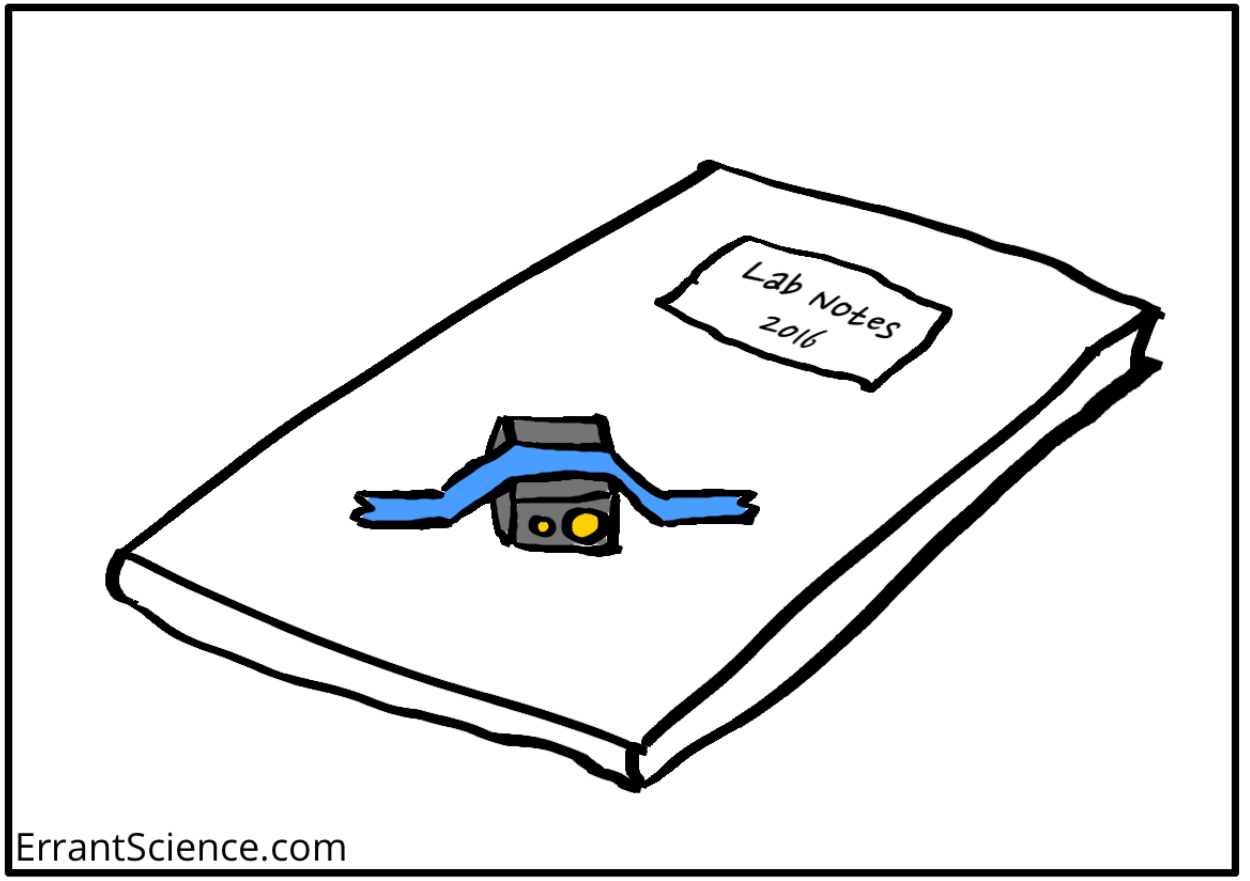
Digital Tool Considerations



- Different situations merit different tools
- Researchers should be using the tools required to produce FAIR data and methods
- Students may be better served with different tools – as the main purpose here is learning
- How can we best prepare our students to go onto be good researchers?

PSDI
PHYSICAL SCIENCES
DATA INFRASTRUCTURE

Examples of Successful Implementations

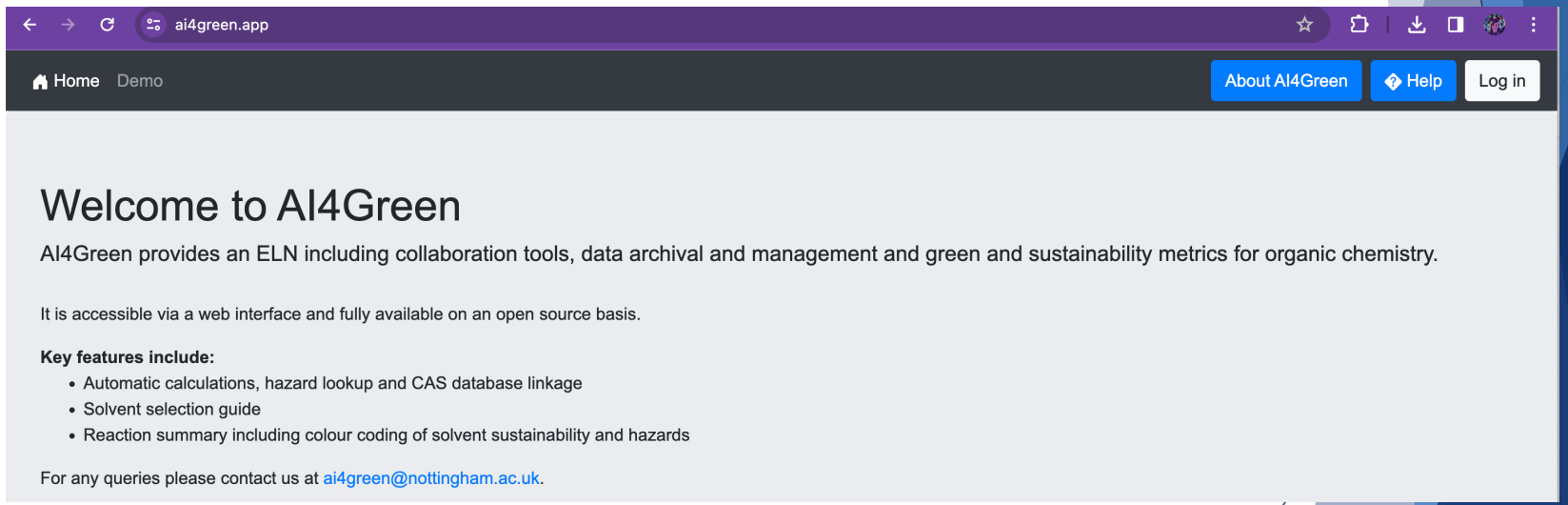


If your electronic lab book looks like this, you're doing it wrong

PSDI
PHYSICAL SCIENCES
DATA INFRASTRUCTURE

Example I – University of Nottingham

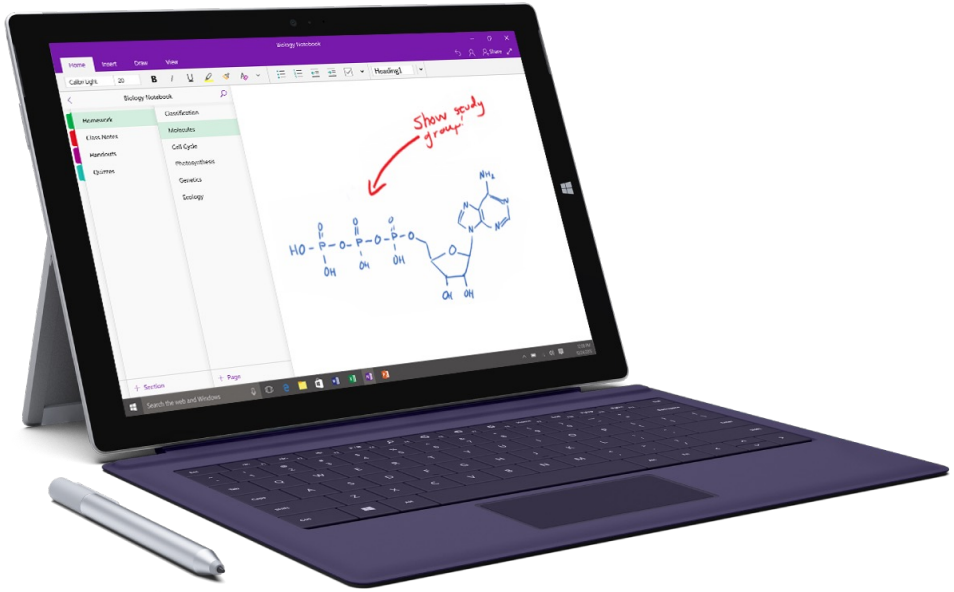
- Undergraduate Labs
  - Tablets for all students
  - All students recording Labs in OneNote
  - Trialing AI4Green Student edition currently
- Postgraduate Labs
  - Computers specifically installed for AI4Green ELN – with well placed monitors
  - Hardwired connections
  - 1 computer per Fumehood
  - No cross contamination of technology



PSDI
PHYSICAL SCIENCES
DATA INFRASTRUCTURE

Example II – Wellington College

- Fully paperless scientific labs
  - Every student must have an MS Surface
  - All students use OneNote
  - Master OneNote for the Teacher
  - Lab benches fully kitted out with power sockets
  - Classroom benches – power sockets installed underneath

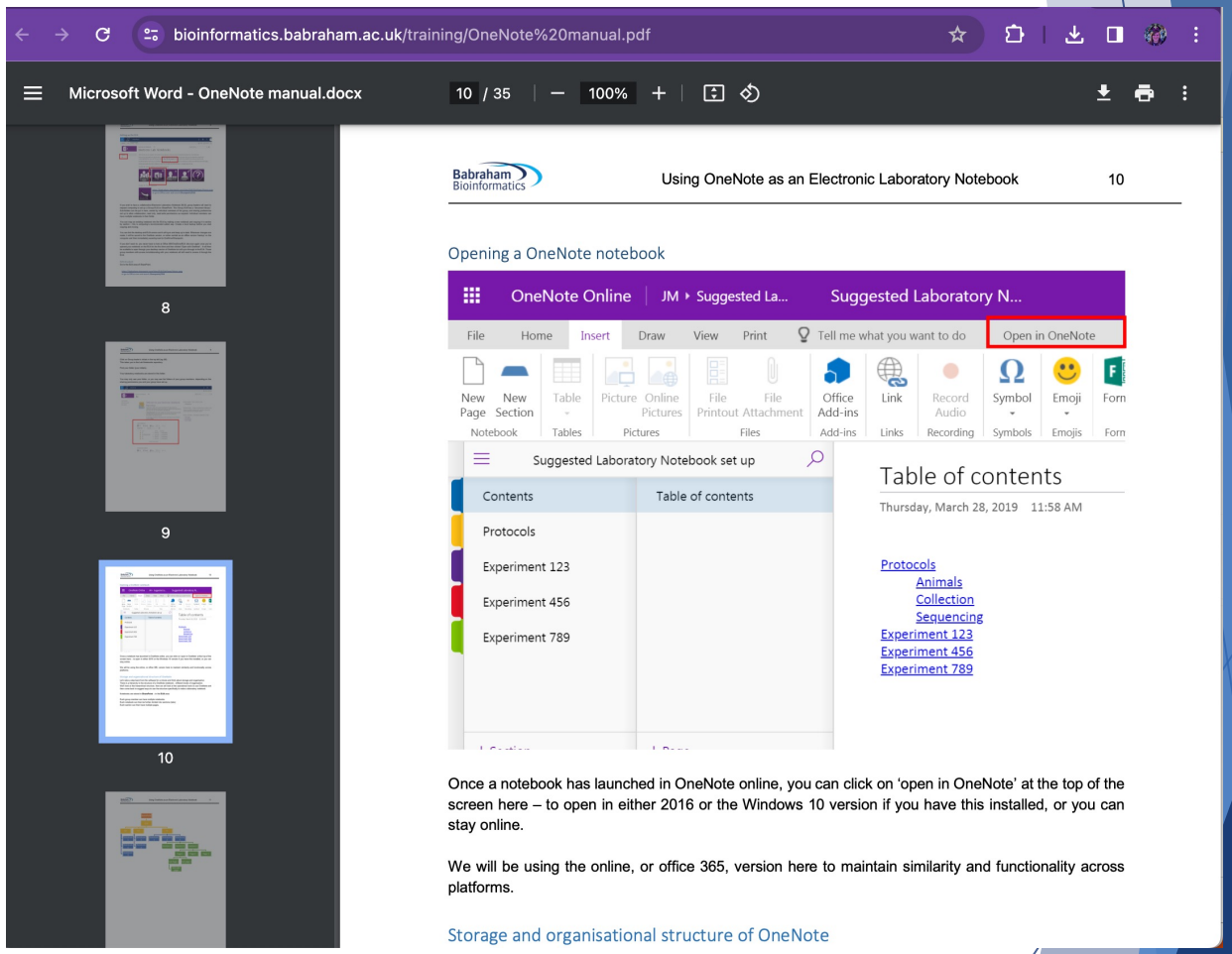


https://www.onenote.com/classnotebook

PSDI
PHYSICAL SCIENCES
DATA INFRASTRUCTURE

Thoughts for the future

- Money & People are the biggest players
- There is never going to be an “ELN to rule them all”
  - But we could implement OneNote for undergraduates (with or without specific ELNs for certain labs)
  - Train them to use digital tools to record their work and instill best practices
  - And implement specific ELNs at Postgraduate/Postdoc level depending on budget/subject



https://www.bioinformatics.babraham.ac.uk/training/OneNote%20manual.pdf

PSDI
PHYSICAL SCIENCES DATA INFRASTRUCTURE

PSDI Services & Research

- Process Recording Service
  - Guidelines on selecting Tools
  - Links to ELNFinder
  - NotebookFinder
  - Guidance on using OneNote as an ELN
- Data Conversion Service
  - Convert between different data formats to enable interoperability
- Metadata Service
  - Generate semantically rich metadata records
  - Generate template READ-ME's
  - Generate license files
- Data Revival Service
  - Scan in paper lab books and get data back in a machine-readable form
- FAIR/Data Sharing Guidelines
  - Guidelines on how to be truly FAIR
  - Exemplars of metadata, supplementary information and data management plans
- Case Studies
  - Different implementations of ELNs
  - Investigating OneNote as a generic ELN
  - Investigating adding semantic/domain knowledge to OneNote

PSDI
PHYSICAL SCIENCES DATA INFRASTRUCTURE

Relevant Publications

- 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
- Kanza, S., 2018. What influence would a cloud based semantic laboratory notebook have on the digitisation and management of scientific research? (Doctoral dissertation, University of Southampton). https://eprints.soton.ac.uk/421045/
- Kanza, S., Gibbins, N. and Frey, J.G., 2019. Too many tags spoil the metadata: investigating the knowledge management of scientific research with semantic web technologies. Journal of cheminformatics, 11(1), p.23. https://doi.org/10.1186/s13321-019-0345-8
- Knight, N.J., Kanza, S., Cruickshank, D., Brocklesby, W.S. and Frey, J.G., 2020. Talk2Lab: The Smart Lab of the Future. IEEE Internet of Things Journal, 7(9), pp.8631-8640. https://doi.org/10.1109/JIOT.2020.2995323
- Kanza, S., Willoughby, C., Bird, C.L. and Frey, J.G., 2021. eScience Infrastructures in Physical Chemistry. Annual review of physical chemistry, 73. https://doi.org/10.1146/annurev-physchem-082120-041521
- Kanza, S., 2021. Guidelines for Chemistry Labs Looking to Go Digital. Digital Transformation of the Laboratory: A Practical Guide to the Connected Lab, pp.191-197. https://doi.org/10.1002/9783527825042.ch13
- Kanza, S., 2021. Understanding and Defining the Academic Chemical Laboratory's Requirements: Approach and Scope of Digitalization Needed. Digital Transformation of the Laboratory: A Practical Guide to the Connected Lab, pp.179-189. https://doi.org/10.1002/9783527825042.ch12
- Kanza, S., 2021. Academic's Perspective on the Vision About the Technology Trends in the Next 5–10 Years. Digital Transformation of the Laboratory: A Practical Guide to the Connected Lab, pp.297-301. https://doi.org/10.1002/9783527825042.ch22
- Kanza, S. and Knight, N.J., 2022. Behind every great research project is great data management. BMC Research Notes, 15(1), pp.1-5. https://doi.org/10.1186/s13104-022-05908-5
- Kanza, S., Willoughby, C., Knight, N.J., Bird, C.L., Frey, J.G. and Coles, S.J., 2023. Digital research environments: a requirements analysis. *Digital Discovery*. https://doi.org/10.1039/D2DD00121G

PSDI
PHYSICAL SCIENCES
DATA INFRASTRUCTURE

Acknowledgements

PSDI Team: Simon Coles, Jeremy Frey, Nicola Knight, Cerys Willoughby, Colin Bird, Ray Whorley, Mark Anderson, Stephen Gow, Samuel Munday, Thomas Allam, Hannah Gittins *(University of Southampton)*, Juan Bicarregui, Barbara Montanari, Brian Matthews, Vasily Bunakov *(Science & Technologies Facilities Council)*

PSDI & Personal Details - Questions

www.psdi.ac.uk

@PSDI_UK

@PSDI_UK

linkedin.com/company/psdiuk

linktr.ee/samanthakanza

Mailing List: *https://www.jiscmail.ac.uk/PSDI*