



# PSDI

PHYSICAL SCIENCES  
DATA INFRASTRUCTURE

## The role of digital note taking for the 21st Century Scientist

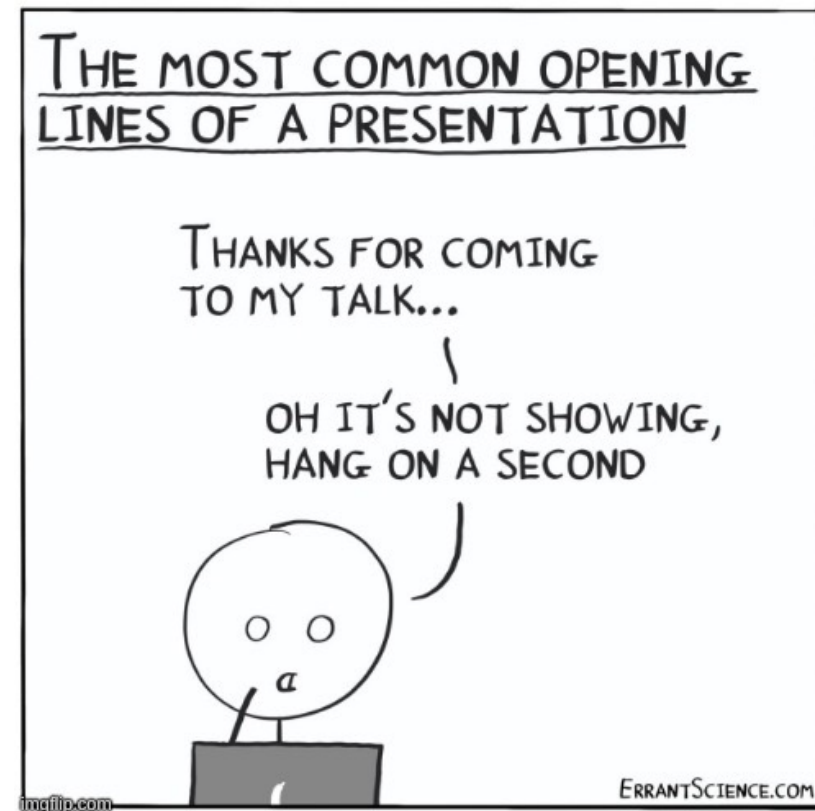
**“The Chemistry Laboratory: Evaluation, Assessment and Research  
Symposium 2024” (CLEAR 24) Global Virtual Symposium**  
**2<sup>nd</sup> May 2024**

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

**Dr Samantha Pearman-Kanza**  
**University of Southampton**

# Presentation Outline

- ▶ About Me & PSDI
- ▶ Scientific Record Keeping
- ▶ Electronic Lab Notebooks
- ▶ Successful Digital Transformations
- ▶ Skills4Scientists
- ▶ Thoughts for the Future

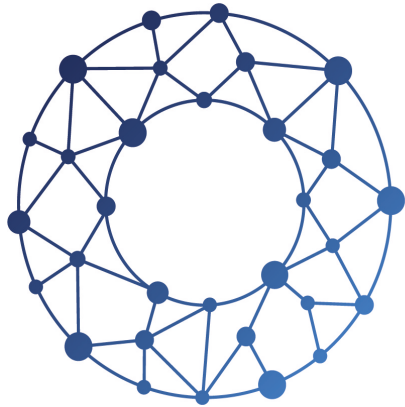


# About Me



- ▶ Senior Enterprise Fellow at University of Southampton
- ▶ Pathfinder Lead & Researcher for PSDI on Process Recording
- ▶ Researcher for AIChemistry Hub on Process Recording
- ▶ Advisory Boards: Future Labs Live, Machines Learning Chemistry
- ▶ Lab Horizons Columnist
- ▶ Research Interests: Semantic Web Technologies, IoT, Research Data Management, Digitisation, Lab of the Future, Paperless Labs
- ▶ @SamiKanza

# About PSDI



**PSDI**  
PHYSICAL SCIENCES  
DATA INFRASTRUCTURE

## Physical Sciences Data Infrastructure

**An Integrated Data Infrastructure for the Physical Sciences**

PSDI aims to accelerate research in the physical sciences by providing a data infrastructure that brings together and builds upon the various data systems researchers currently use.



Through PSDI researchers will be able to:

- ▶ Find and Access to reference quality data from commercial and open sources
- ▶ Combine data from different sources
- ▶ Share data, software and models including experimental and simulation data
- ▶ Use AI to explore data
- ▶ Learn how to make the results of their research open and FAIR




# How did I end up here?

**BMC** Part of Springer Nature

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## Journal of Cheminformatics

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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](#)

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#### 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

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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 Kwock](#)



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.*, *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

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#### Subjects

[Lab life](#) [Research management](#) [Research data](#)

[Technology](#)



Personal Photograph of Dr Samantha Pearman-Kanza

# Digital Research

## LITERATURE REVIEW

Systematic literature review of different aspects of digital technologies in the Physical Sciences

1

2

## SOFTWARE INVESTIGATIONS

- Investigate usage of non ELN software for Chemists
  - ELN Survey for Physical Sciences Community
- ELN Landscape assessment

3

4

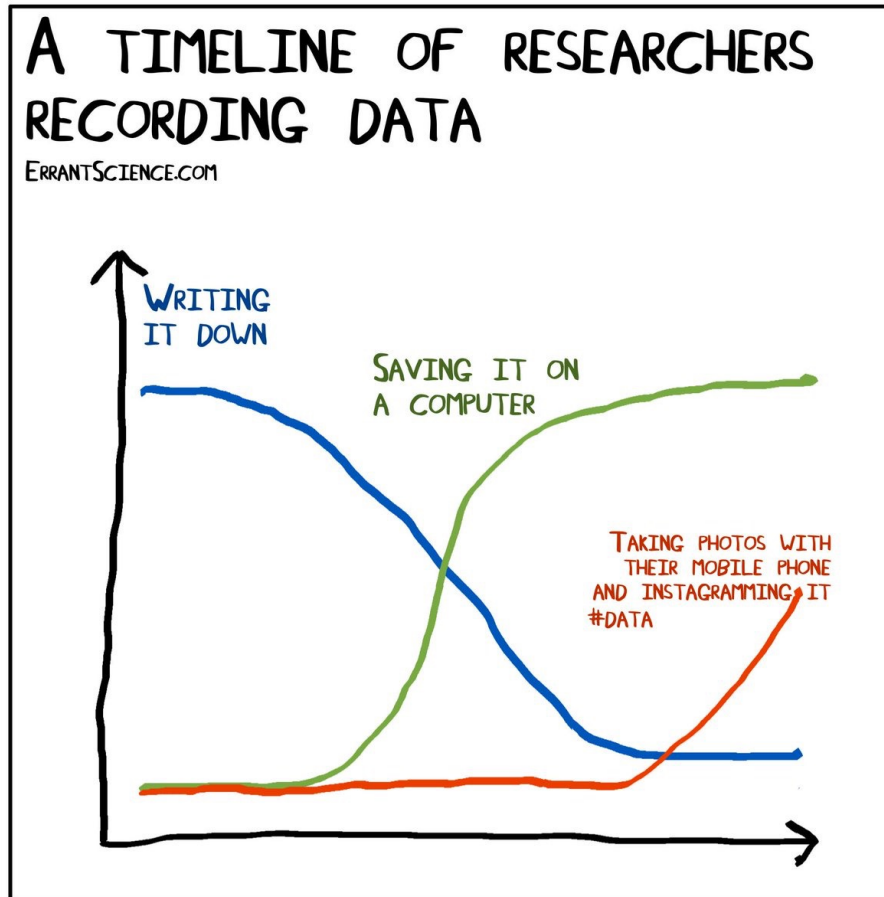
## QUALITATIVE RESEARCH

- Research to understand current landscape of digitisation and use of technology
- Focus Groups (Physics, Chemistry, Biology)
- Ethnography in chemistry laboratories
- Surveys of Physical Sciences Community
- AI4Green Case Study & Lab Observations
- OneNote Case Study & Lab Observations

## TECHNICAL PROTOTYPES

- Semantic tagging and annotation of scientific documents
- Smart Lab prototyping
- Investigations of how to implement Microsoft Ecosystem into laboratories

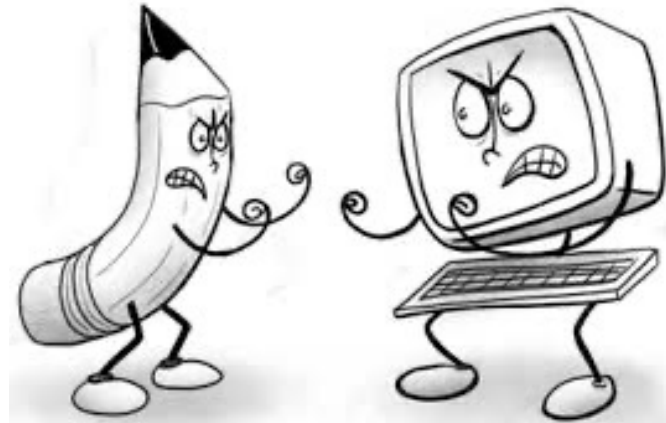
# Scientific Record Keeping



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

# 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





# 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>

# 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

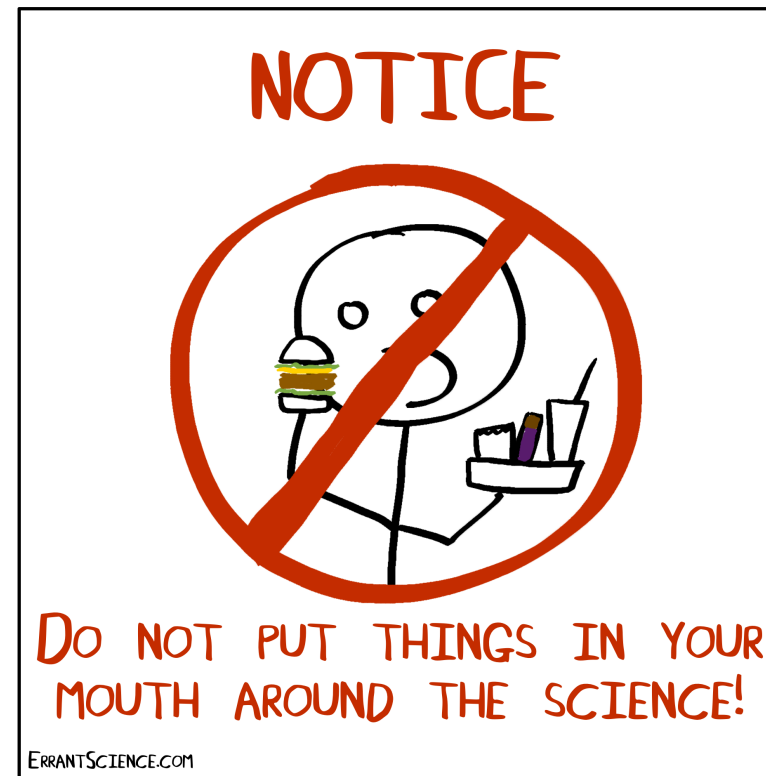
- ▶ Accessible from multiple locations
- ▶ Searchable
- ▶ Easy to backup
- ▶ Easy to share data
- ▶ Data is quickly retrievable
- ▶ Can be used by multiple people at once

## Disadvantages

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

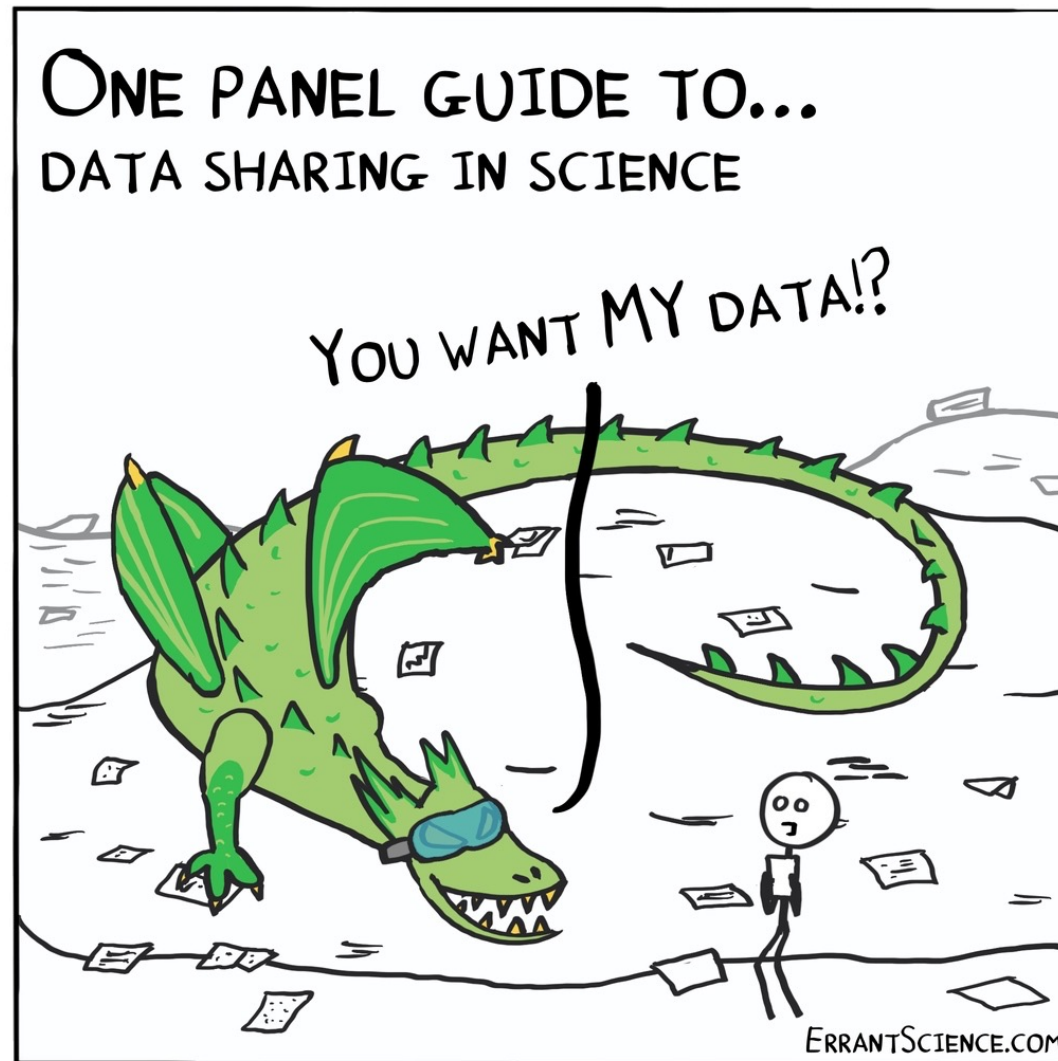
# Barriers to ELNs

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



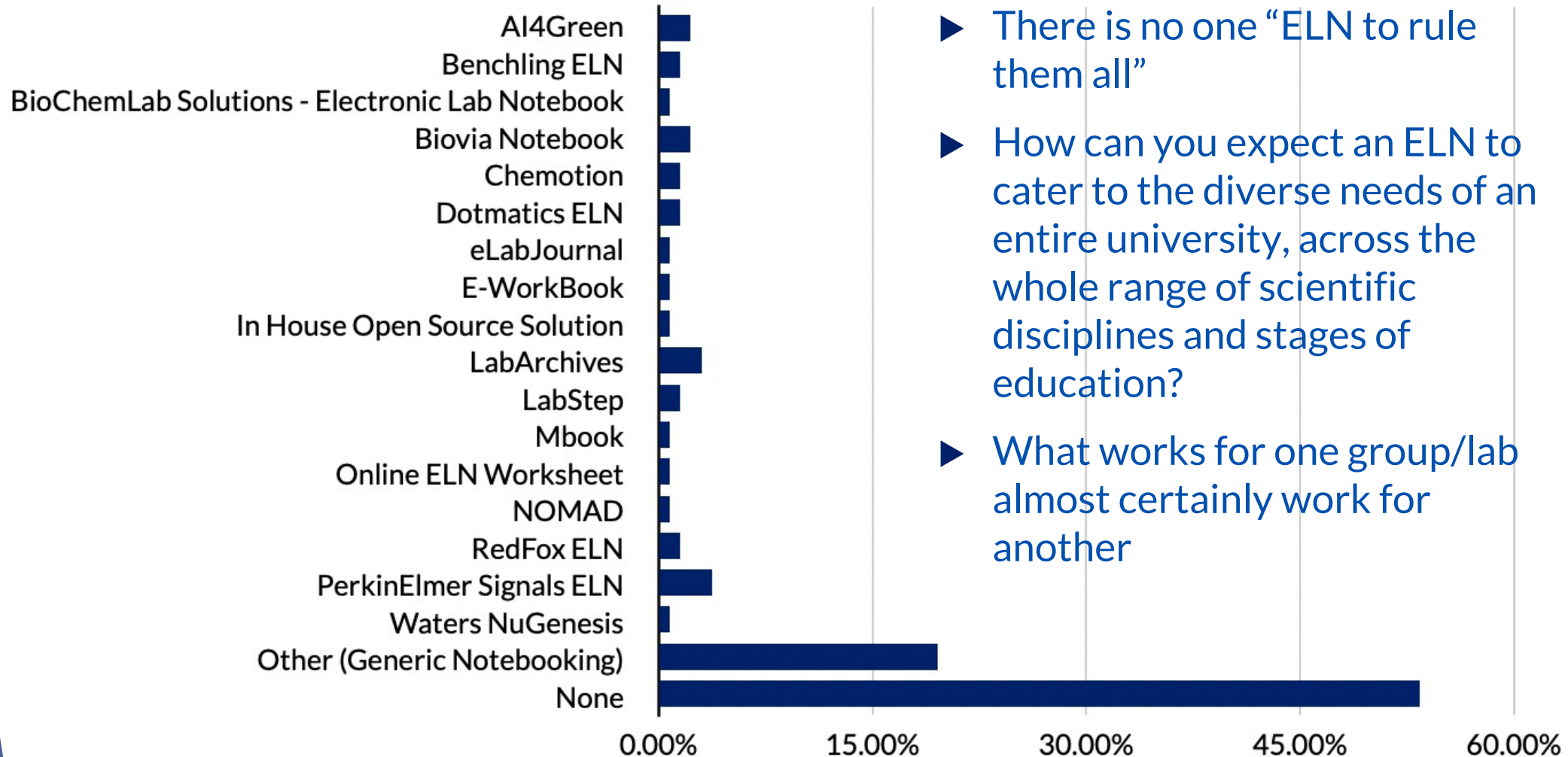
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# Why does this matter?





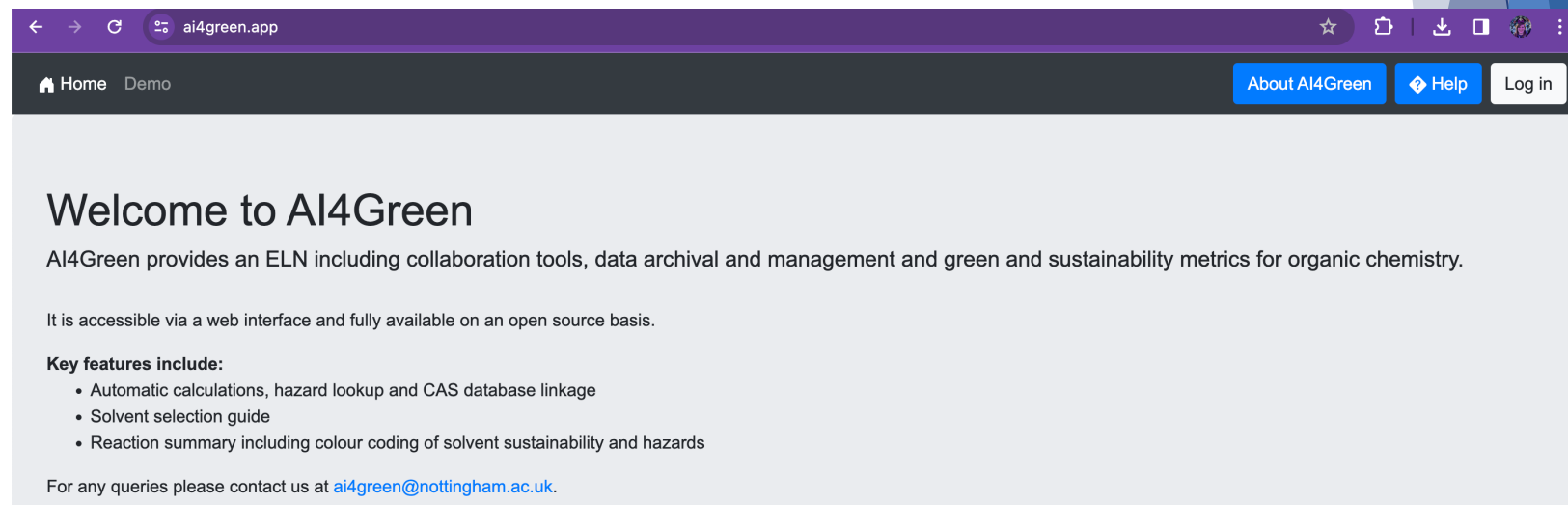
# Current state of play



- ▶ 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

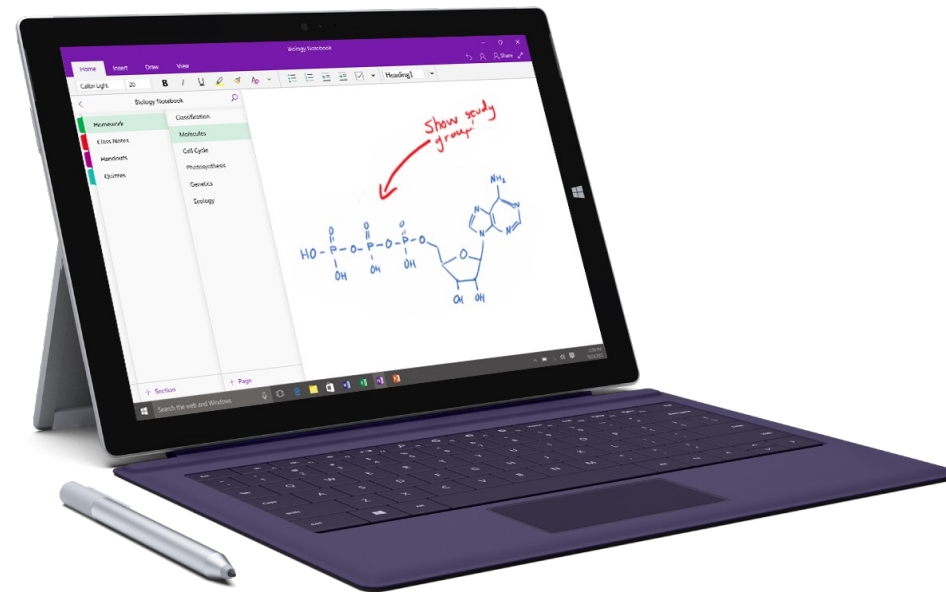
# Example I – University of Nottingham

- ▶ 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



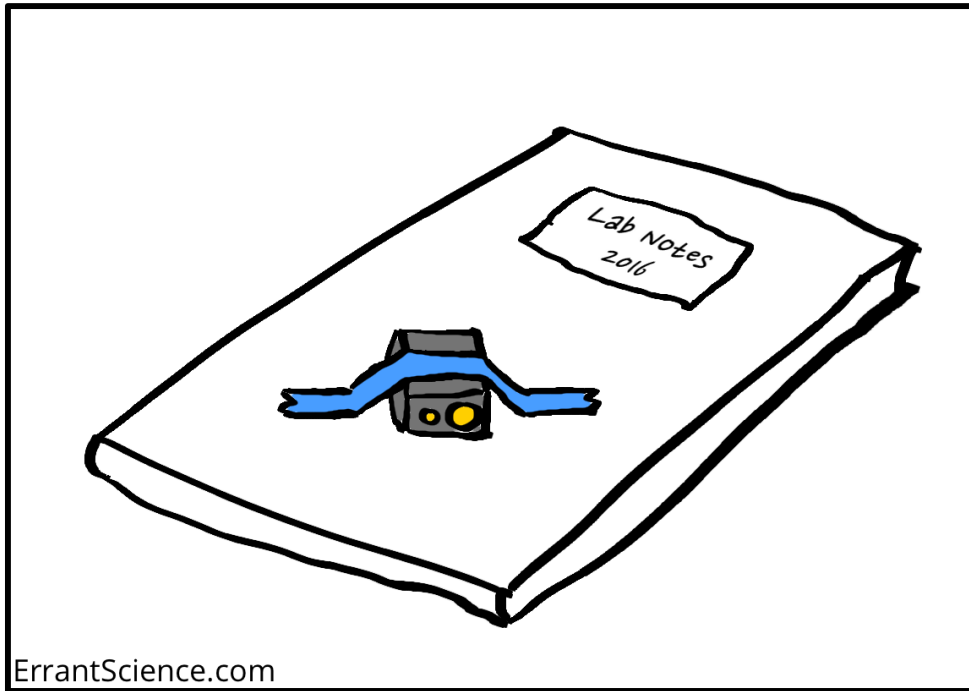
# Example II – Wellington College

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



<https://www.onenote.com/classnotebook>

# Digital Tool Considerations for Undergraduates



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

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- ▶ Different situations merit different tools
- ▶ Researchers should be using the tools required to produce FAIR data and methods, Undergrads need to learn these principles
- ▶ Students may be better served with different tools – as the main purpose here is learning
- ▶ Don't ruin learning with automation!
- ▶ How can we best prepare our students for their future careers?



# Skills4Scientists

## Technical / Scientific Skills

- ▶ Introduction to Python
- ▶ GitHub/Version Control
- ▶ Using the Command Line
- ▶ Good Coding Practices
- ▶ Machine Learning
- ▶ Intro to Cheminformatics



## Careers

- ▶ CV Talks
- ▶ Careers Panels
- ▶ Cultivating your web presence

## Data Skills

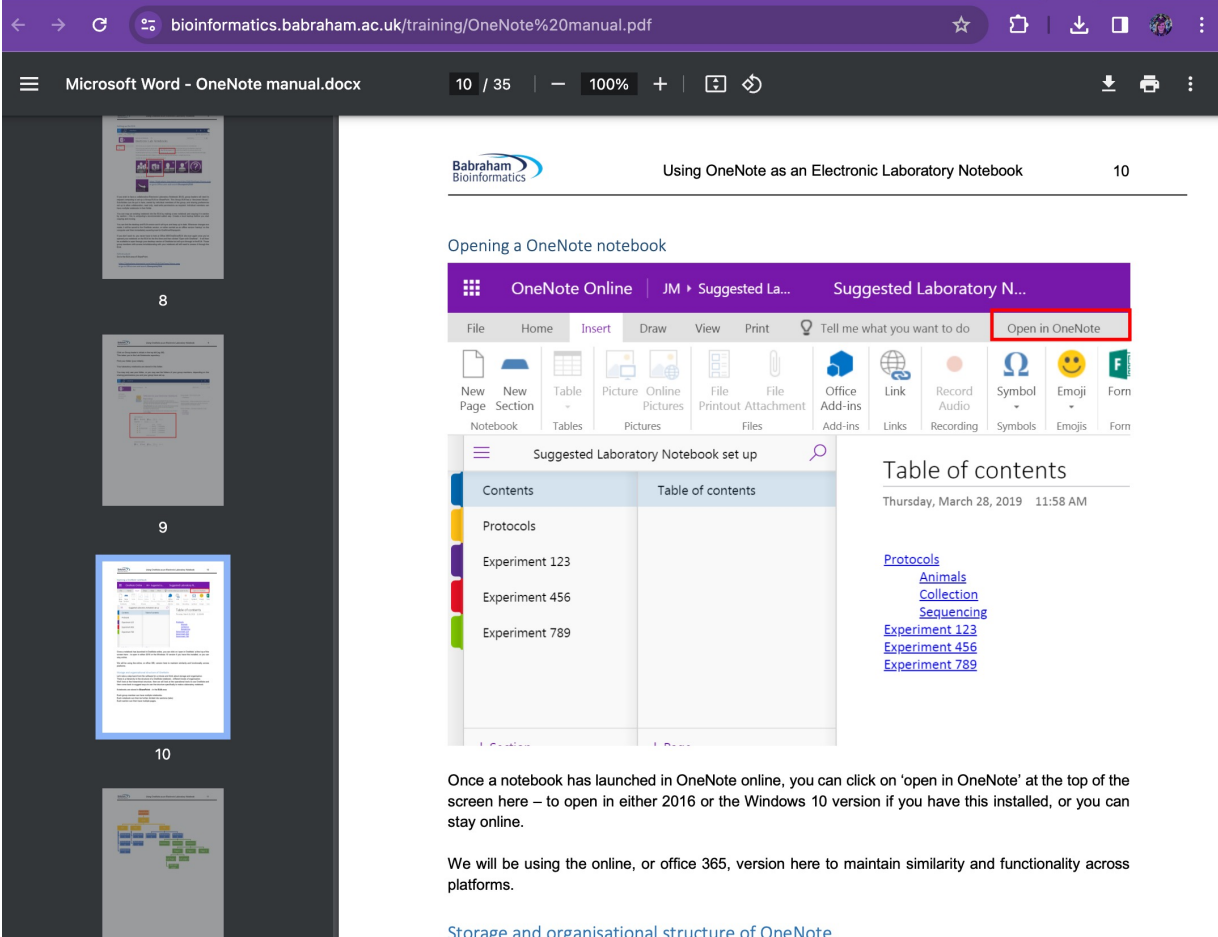
- ▶ Research Data Management
- ▶ Collaborative Data Management
- ▶ FAIR Data & Metadata
- ▶ Databases
- ▶ Semantic Web Technologies
- ▶ Research & Data Ethics

## Dissemination/Communication Skills

- ▶ Presentations
- ▶ Reports
- ▶ Posters
- ▶ LaTeX/Overleaf

# 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/MS Tools 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
- ▶ Integrating new systems at the beginning of a students journey is much easier and less disruptive



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

Microsoft Word - OneNote manual.docx 10 / 35 100%

Babraham Bioinformatics Using OneNote as an Electronic Laboratory Notebook 10

Opening a OneNote notebook

OneNote Online JM ▶ Suggested La... Suggested Laboratory N...

File Home Insert Draw View Print Tell me what you want to do Open in OneNote

New Page New Section Table Picture Online File File Office Link Record Symbol Emoji F  
Notebook Tables Pictures Printout Attachment Add-ins Links Recording Symbols Emojis Forn

Suggested Laboratory Notebook set up

Contents	Table of contents
Protocols	
Experiment 123	
Experiment 456	
Experiment 789	

Table of contents

Thursday, March 28, 2019 11:58 AM

[Protocols](#)  
[Animals](#)  
[Collection](#)  
[Sequencing](#)  
[Experiment 123](#)  
[Experiment 456](#)  
[Experiment 789](#)

Once a notebook has launched in OneNote online, you can click on 'open in OneNote' at the top of the screen here – to open in either 2016 or the Windows 10 version if you have this installed, or you can stay online.

We will be using the online, or office 365, version here to maintain similarity and functionality across platforms.

Storage and organisational structure of OneNote

# Relevant Talks

- ▶ Kanza, S. (2022, June 7). The effects of COVID-19 on the digitisation of Scientific Research - Presentation at Future Labs Live 2022. Future Labs Live 2022 (FLL2022), Basel. Zenodo. <https://doi.org/10.5281/zenodo.10118139>
- ▶ Kanza, S. (2022, October 4). To Digitisation And Beyond! The Digitisation Requirements Of A 21st Century Scientist - Presentation at Drug Discovery World 2022. Drug Discovery World 2022 (DDW2022), London. Zenodo. <https://doi.org/10.5281/zenodo.10142544>
- ▶ Kanza, S. (2022, December 6). Technical and Data Requirements of Digitalising Scientific Research - Presentation at Smart Labs & Automation 2022. Smart Labs & Automation, London. Zenodo. <https://doi.org/10.5281/zenodo.10142749>
- ▶ Kanza, S. (2023, January 25). The Digitisation of Scientific Research: Requirements, Barriers and Logistics - Presentation at Lab of the Future 2023. Lab of the Future 2023, Online. Zenodo. <https://doi.org/10.5281/zenodo.10142604>
- ▶ Kanza, S. & Knight, N. (2023, March 29). Process recording and digitisation requirements for the 21st century scientist - Presentation for ACS Spring 2023. ACS SPRING 2023 Crossroads of Chemistry (ACS SPRING 2023), Indianapolis, IN & Hybrid. Zenodo. <https://doi.org/10.5281/zenodo.10144147>
- ▶ Kanza, S. (2023, May 31). ELNs are Dead! Long Live ELNs! - Presentation at Future Labs Live 2023. Future Labs Live 2023 (FLL2023), Basel. Zenodo. <https://doi.org/10.5281/zenodo.10138225>
- ▶ Kanza, S. (2023, August 13). We don't talk about Semantic Web Technologies - Presentation at ACS Fall 2023. ACS FALL 2023 Harnessing the Power of Data (ACS FALL 2023), San Francisco, CA & Hybrid. Zenodo. <https://doi.org/10.5281/zenodo.10149599>
- ▶ Kanza, S. (2023, August 14). Electronic Lab Notebooks and Beyond! The evolution of process recording tools for scientific research - Presentation at ACS Fall 2023. ACS FALL 2023 Harnessing the Power of Data (ACS FALL 2023). Zenodo. <https://doi.org/10.5281/zenodo.10149499>
- ▶ Pearman-Kanza, S. (2023, November 1). To the well organised FAIR dataset, re-use is but the next great adventure - Presentation at Lab Innovations 2023. Lab Innovations 2023, NEC, Birmingham. Zenodo. <https://doi.org/10.5281/zenodo.10119611>
- ▶ Pearman-Kanza, S. (2023, December 7). How can we combat heterogeneous, unfair and disparate data in digital chemistry? Presentation at the ChemSpider Webinar Series. ChemSpider Webinar Series: Challenges and opportunities for digital chemistry data, Online. Zenodo. <https://doi.org/10.5281/zenodo.10417786>
- ▶ Pearman-Kanza, S. (2024, March 13) Electronic Lab Notebooks and Beyond! The evolution of process recording tools for scientific research'. RSC Historical Group Open Meeting, Zenodo <https://doi.org/10.5281/zenodo.10818945>

# 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>



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# PSDI & Personal Details - Questions

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