Mitigating Barriers and Maximising Opportunities in Chemistry Research Data Management

John Jolliffe, Samantha Pearman-Kanza, Nicola Knight

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Outline

- Who are NFDI4Chem and PSDI?
- Current landscape of Chemistry Research Data Management (RDM)
- Barriers to and Opportunities in Chemistry RDM
- International Chemistry RDM Co-operations

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Why are we here?
Who are we?

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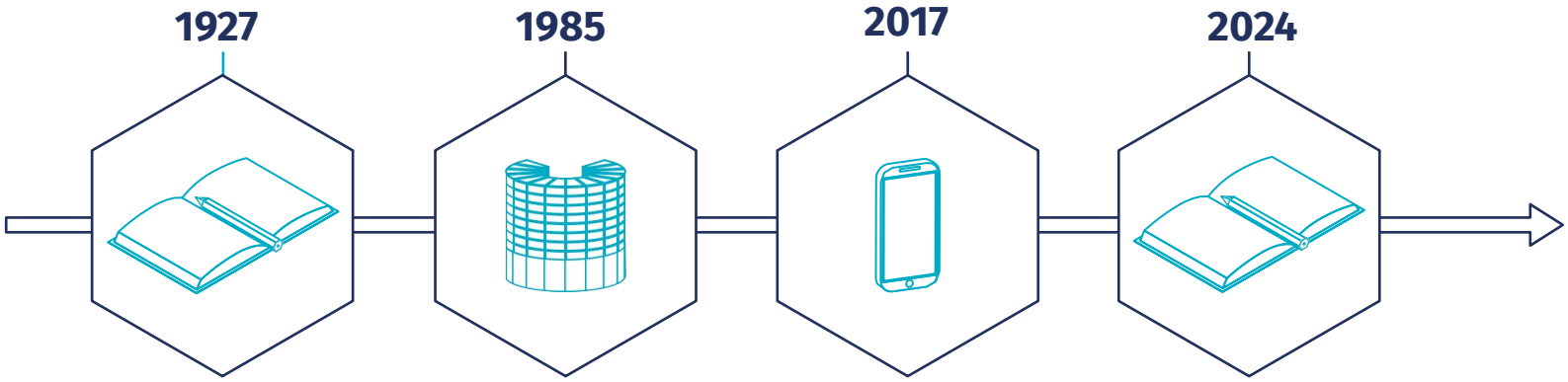
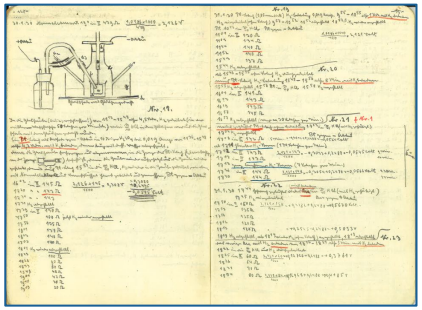
Speed of Evolution





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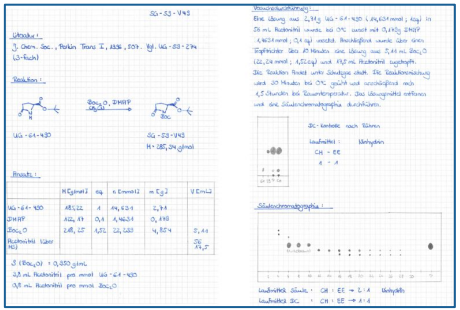
1.9 GFlops
244 MHz CPU Speed

IPhone 8
325.0 GFlops
2.39 GHz CPU Speed



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National Research Data Infrastructure

- German National Research Data Infrastructure
- Founded in 2018 – funded by federal government and states
- **Main goal:** Improvement and creation of Research Data Infrastructure & Management.
- Provision of tools, trainings and initiation of cultural change.
- Part of federal governments digitalisation strategy
- Different consortia representing different scientific disciplines

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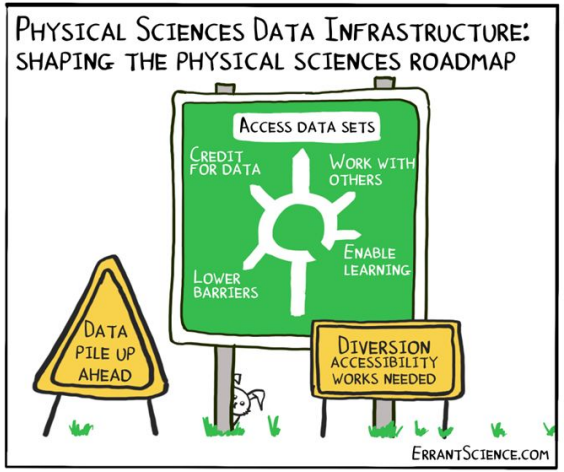
DFG Deutsche Forschungsgemeinschaft

Composition of NFDI4Chem

Physical Sciences Data Infrastructure



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- Funded by UKRIs ‘Digital Research Infrastructure’ fund
- Pilot in 2021, development activities started late 2022
- Creating connections between existing experimental and computational facilities
- Not just technology components, but skills, culture and community
- At the core supporting Chemistry, Materials and related disciplines, but interfacing with Life, Medical, Engineering and Environmental Sciences

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Who is involved in PSDI (so far)

CCDC advancing structural science

Cardiff University / Prifysgol Caerdydd

CatalysisHub

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DCC

University of Sheffield | Henry Royce Institute

Loughborough University

UKRI Science and Technology Facilities Council – Scientific Computing

University of Southampton

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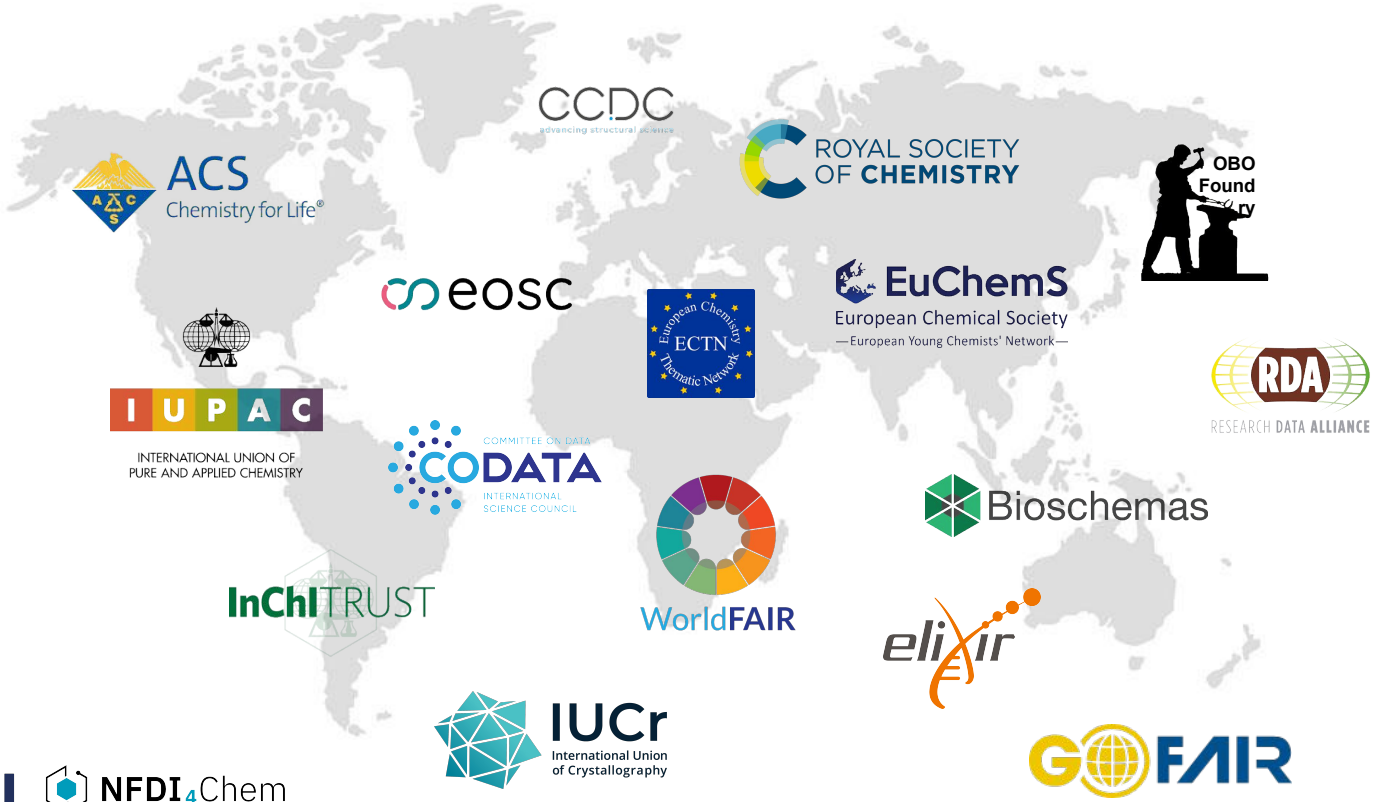
International Network of PSDI and NFDI4Chem



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What is the status Quo for Research Data in Chemistry?

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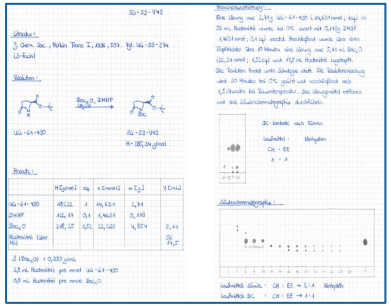
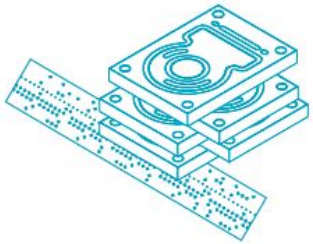
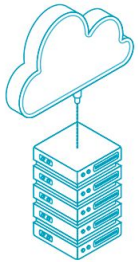
Status Quo

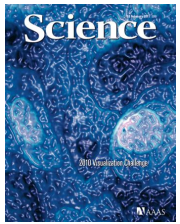
Analogue / Digital

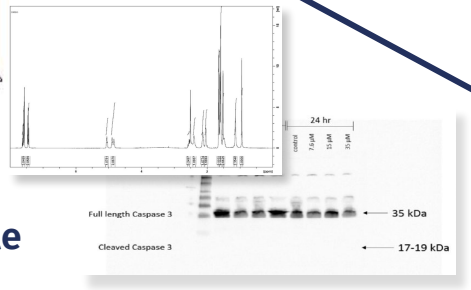




Digital







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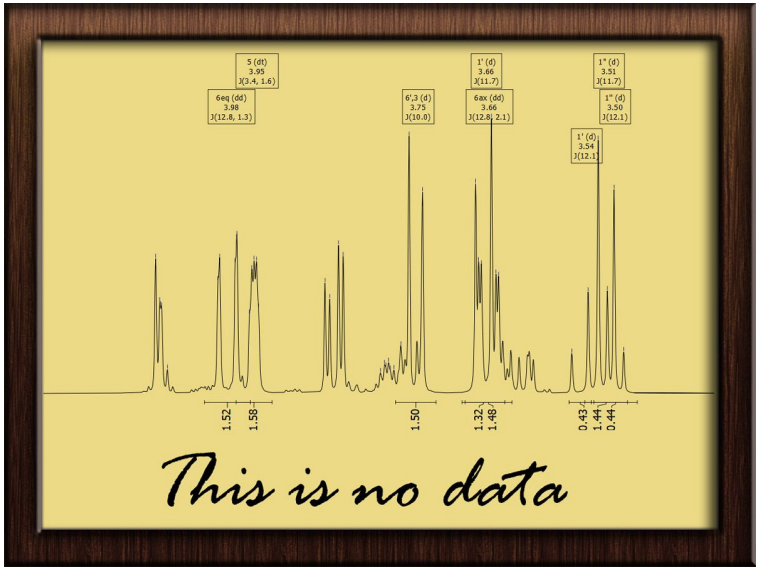
Status Quo



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Worst Case

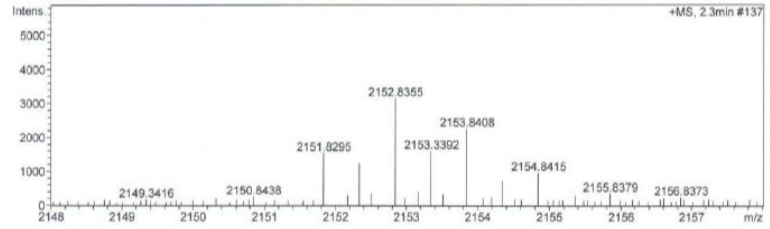
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	[redacted]20328.d	Acquisition Date	5/13/2020 10:10:26 PM
Method	20150915.m	Operator	[redacted]
Sample Name	2015110-7-76	Instrument / Ser#	maXis 4G 21240
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	220 °C
Scan Begin	300 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	2900 m/z	Set Collision Cell RF	2000.0 Vpp	Set Divert Valve	Waste



Meas. m/z # Formula Score m/z err [ppm] Mean err [ppm] mSigma rdb e⁻ Conf N-Rule

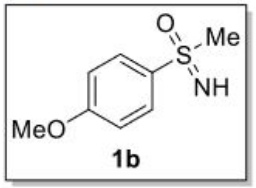
$C_{124}H_{128}O_{32}$ $[M+Na]^+$

2151.828492

2152.831487

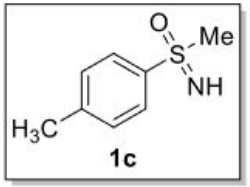
2151.8295

Looks neater but still worst case



1b

1-Methoxy-4-(*S*-methylsulfonimidoyl)benzene (1b). Isolated in 95% yield (907.1 mg, 4.90 mmol) as a faint yellow soild. ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.85 (d, J = 8.8 Hz, 2H), 7.11 (d, J = 8.8 Hz, 2H), 4.05 (s, 1H), 3.84 (s, 3H), 3.02 (s, 3H). ^{13}C NMR (151 MHz, DMSO-d_6) δ 162.3, 135.7, 129.4, 114.1, 55.6, 46.3.



1c

1-Methyl-4-(*S*-methylsulfonimidoyl)benzene (1c). Isolated in 72% yield (608.4 mg, 3.60 mmol) as a faint yellow oil. ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.81 (d, J = 8.0 Hz, 2H), 7.40 (d, J = 7.6 Hz, 2H), 4.12 (s, 1H), 3.03 (s, 3H), 2.39 (s, 3H). ^{13}C NMR (151 MHz, DMSO-d_6) δ 143.2, 141.7, 129.9, 127.8, 46.3, 21.4.

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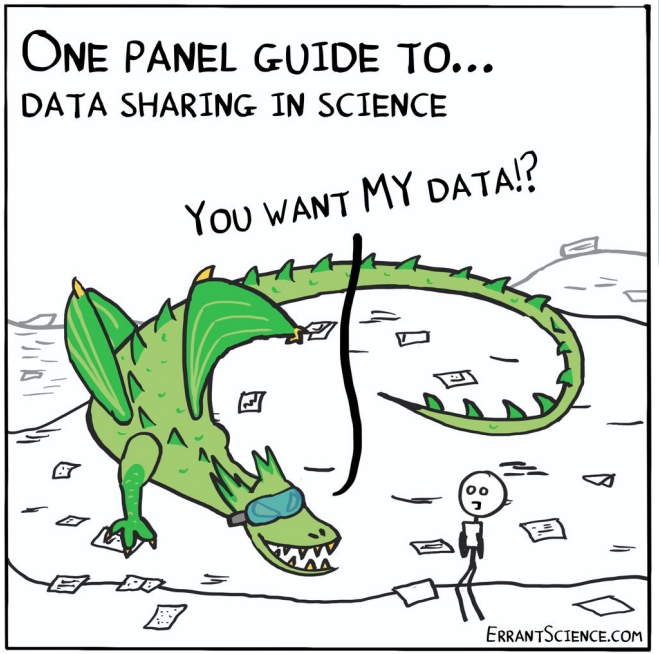
More examples of poor data sharing

- Data available on request
- A spreadsheet called results.xlsx with no description
- Method as in Smith et al 2016, where that paper references White et al 2014, which references another paper…
- 1 file with all the information together and no description
- Compound identifiers not included with the data files
- And more…



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results.xlsx

Data availability

The data that support the findings of this study are available from the corresponding authors upon reasonable request.

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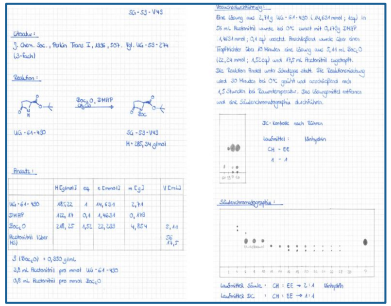
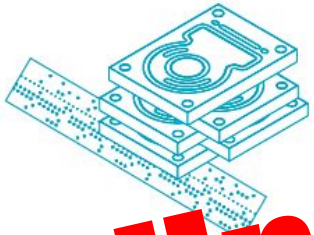
Status Quo

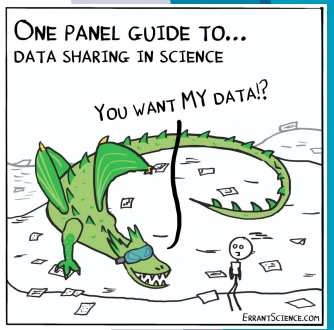
Analogue / Digital



results.xlsx

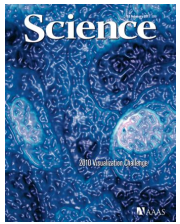


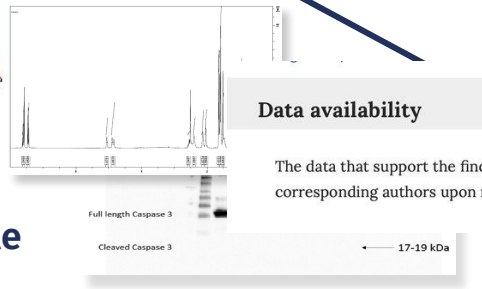
Digital



UnFAIR

Findable
Accessible
Interoperable
Reusable





Not machine readable

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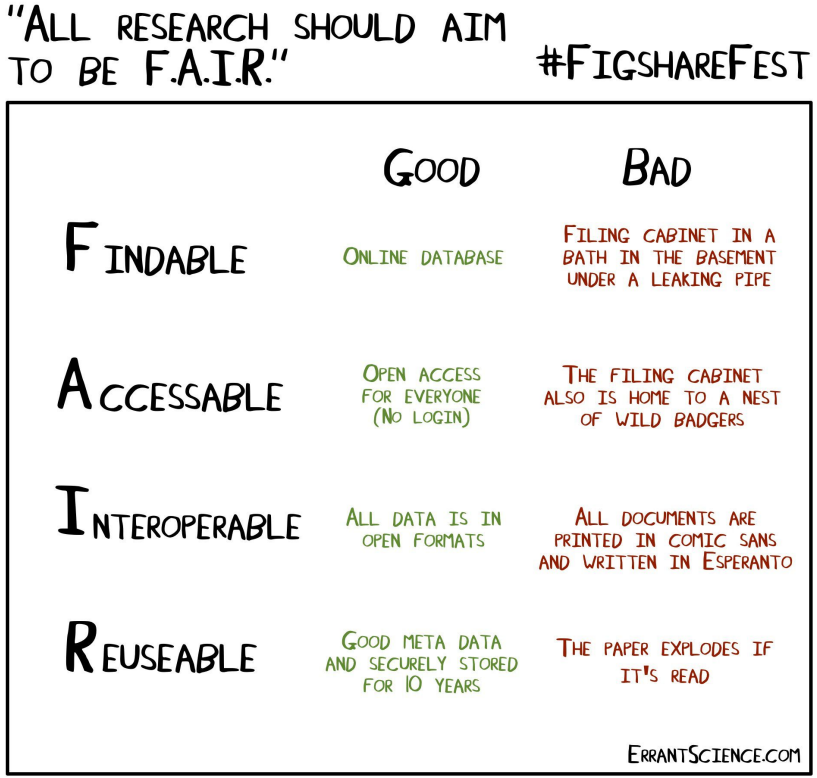
What does FAIR mean?



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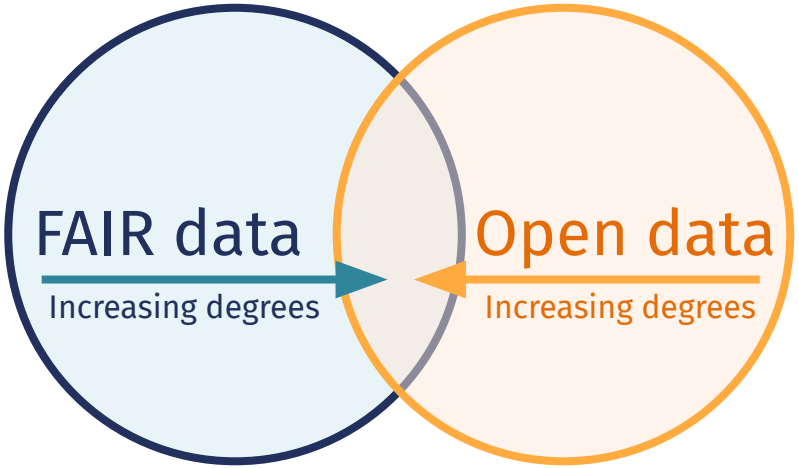
FAIR and Open

- Not all Open Data are FAIR, not all FAIR data are necessarily open

Findable
Accessible
Interoperable
Reusable



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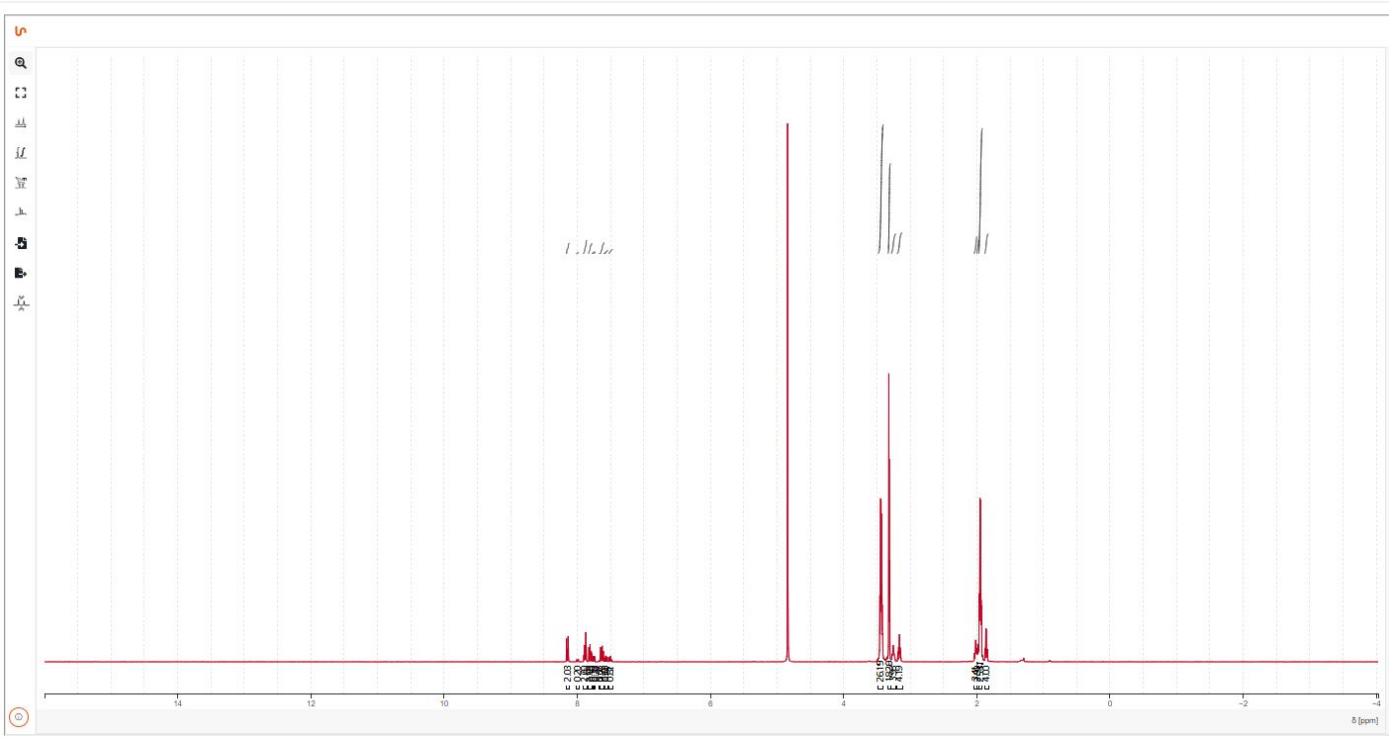
An example of FAIR Data: 1H-NMR Spectrum



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F is for Findable

- To be Findable:
  - It needs to exist
  - But existing ≠ findable
  - Provide your users with pointers!
  - Structured metadata according to standardised metadata schemata to make it findable:

    → Metadata answers the “w” questions: who did what, how, when and where?

- Example for NMR: Dataset can be found via persistent identifier such as a doi (digital object identifier)

  https://dx.doi.org/10.14272/KDWZDHRURBJEIN-UHFFFAOYSA-N/CHMO0000593

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A is for Accessible

- To be accessible:
  - Human and machine accessible
  - What should and shouldn't be accessible?
  - If access is restricted or complex, have you provided relevant information?
  - Technically accessible ≠ Easily accessible
- Example for NMR:
  - Dataset is published online in data repositories
  - Ideally, in data repositories where all NMR data are published in a standardised way

Chemotion Repository

nmrXiv

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I is for Interoperable

- To be interoperable
  - Consider your data standards
  - Use Common and Shared Vocabularies
    - For Data and Metadata
  - Use Ontologies/Knowledge Graphs to the best of their potential

- Example for NMR:
  - Data is published in non-proprietary, open data format such as jcamp.dx

~~*.mnova~~ *.jdx

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What is JCAMP-DX

- IUPAC standard format family for spectral data exchange
- Non-proprietary, open data format
- Text-based format for spectroscopic data
- Started for Infrared spectroscopy
- Expanded to include **NMR** and other methods
- In principle, any two-dimensional data can be depicted with JCAMP-DX

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```

R is for Re-useable

- This isn't JUST about the data! You need to consider:
  - Metadata, Data, Tools, Code, Methods, Context
  - How could/would your work be re-used, replicated, reproduced or repurposed
    - Re-use – re-use the data 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 for a new purpose
- Example for NMR:
  - Re-use of data is clearly defined via an appropriate CC-license such as CC-BY-4.0

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This is only the tip of the "R" Iceberg

Why FAIR Data and how do we get there?

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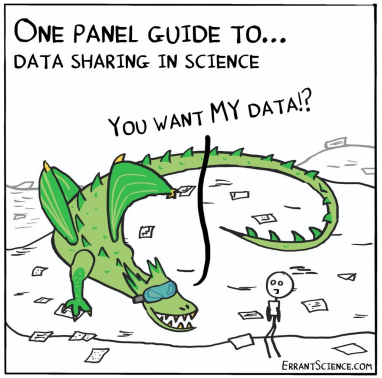
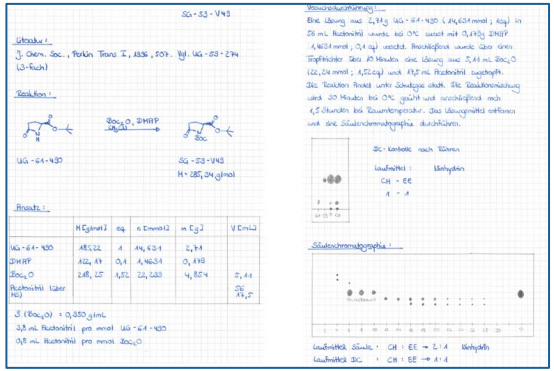
Our Vision





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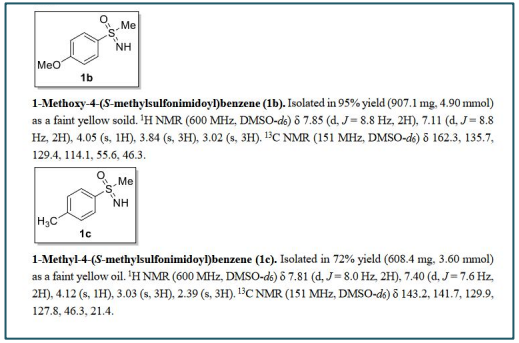
results.xlsx



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FAIR?

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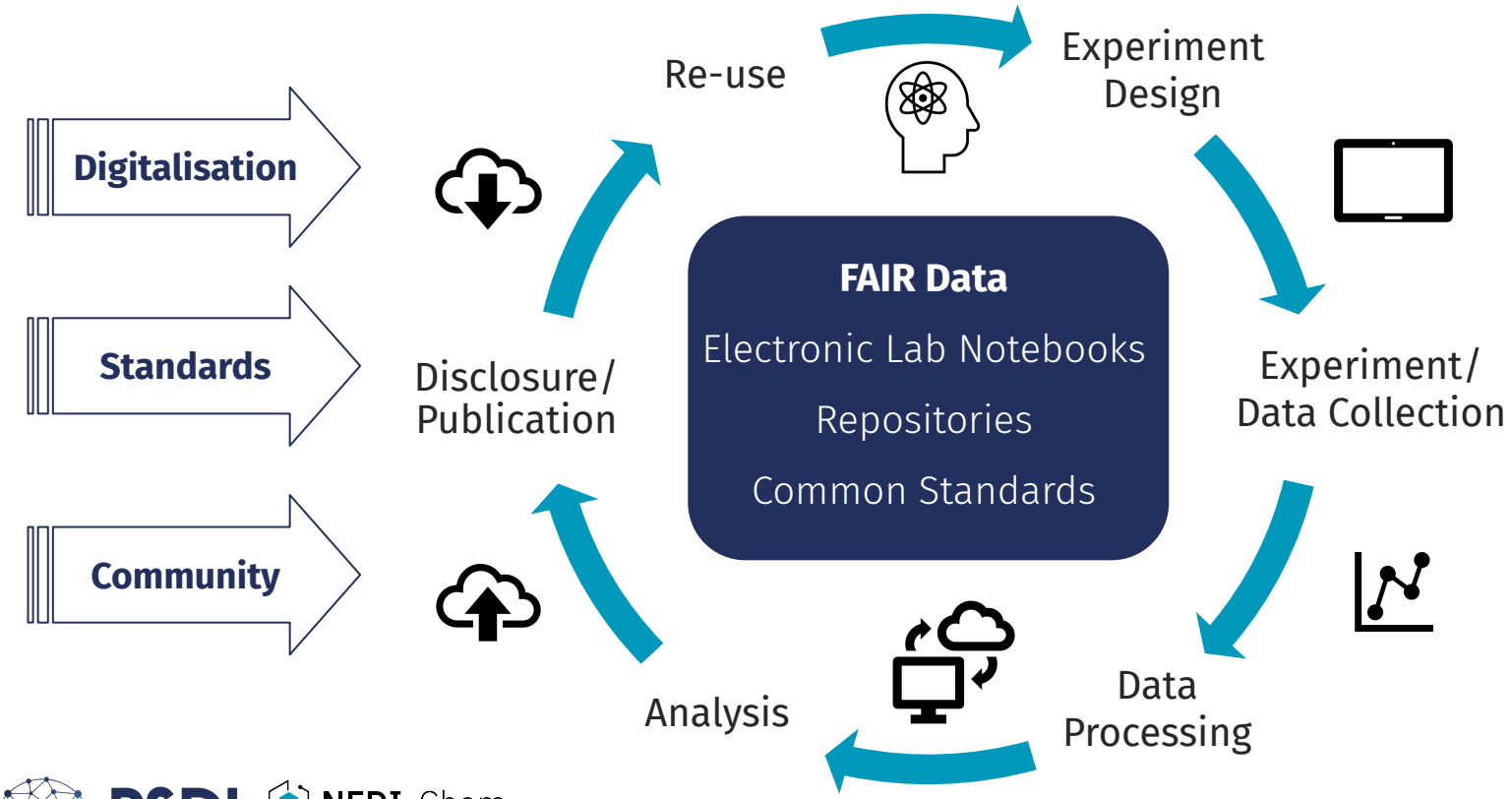
NFDI4Chem ENHANCE YOUR DATA.

Our Vision: All chemists publish FAIR data



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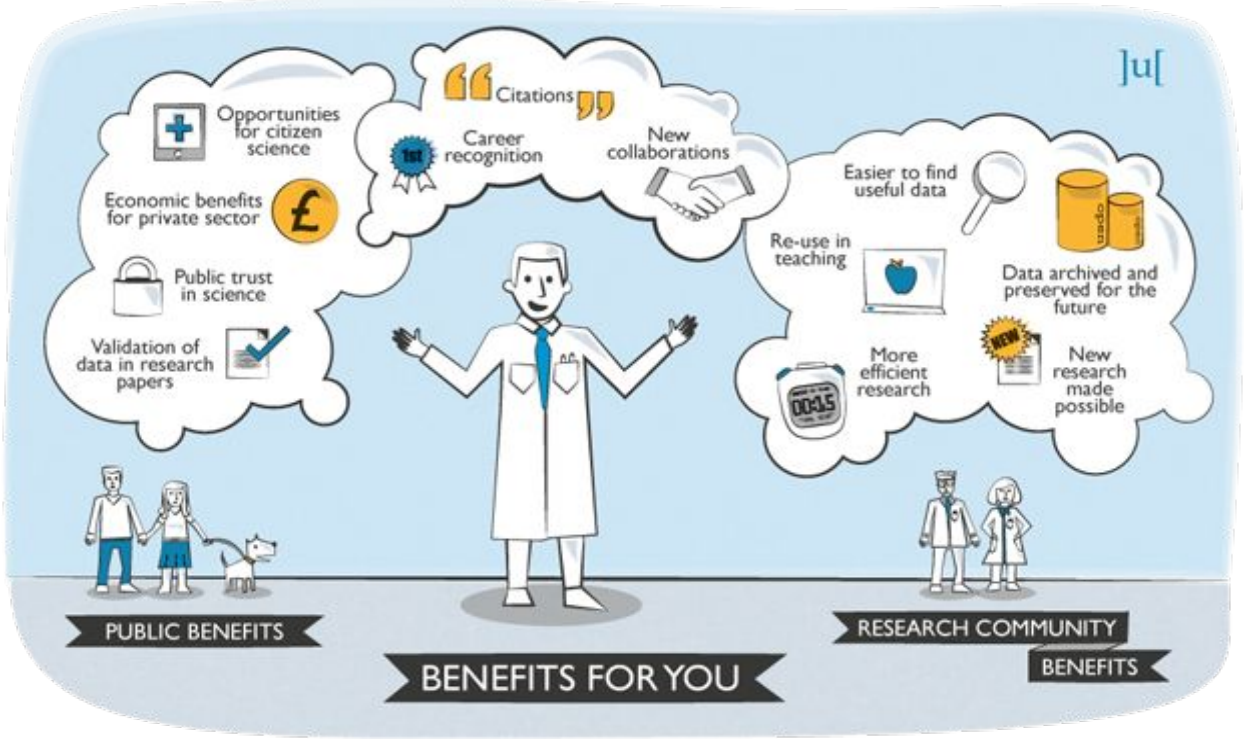
Why FAIR Data?



https://www.slideshare.net/brianhole/the-journal-of-open-archaeology-data-and-prime-incentivising-open-data-archiving

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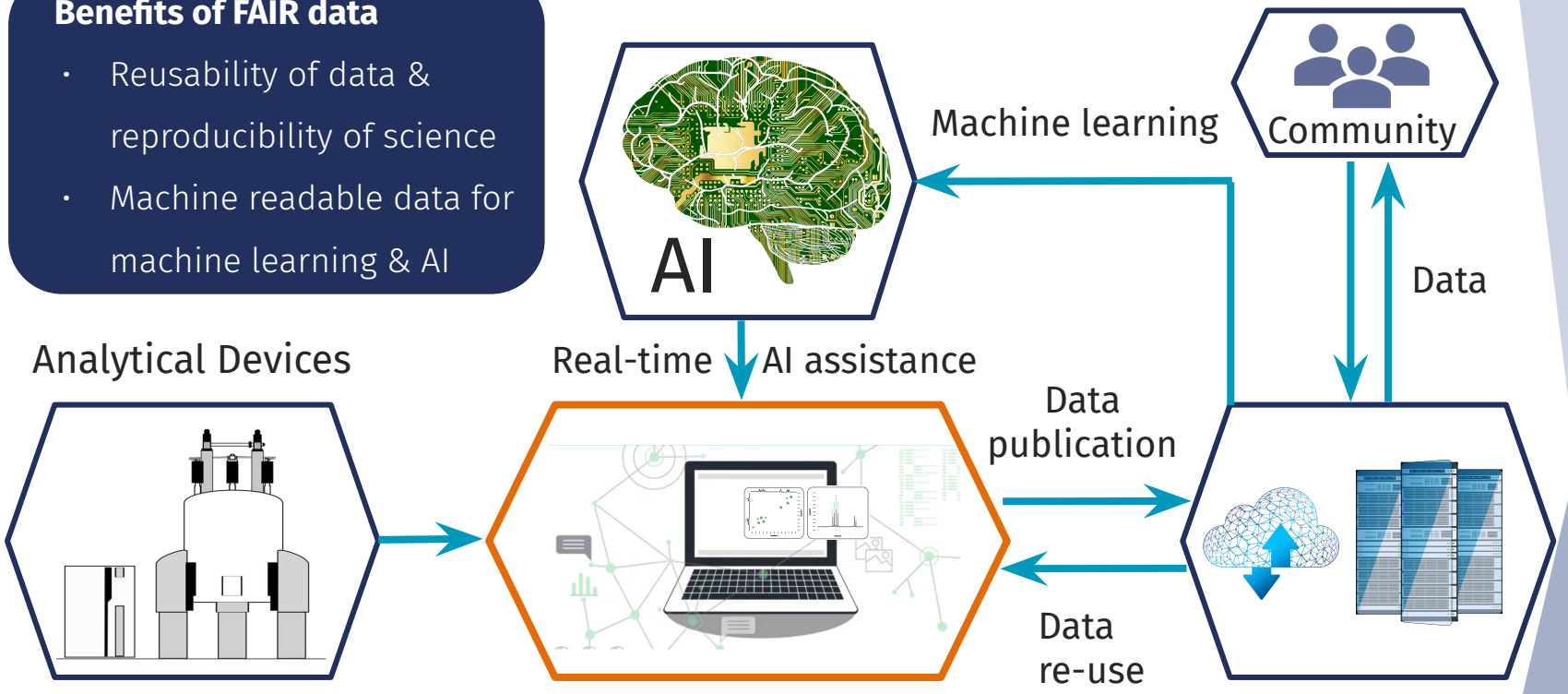
Why FAIR Data?

Benefits of FAIR data

- Reusability of data & reproducibility of science
- Machine readable data for machine learning & AI



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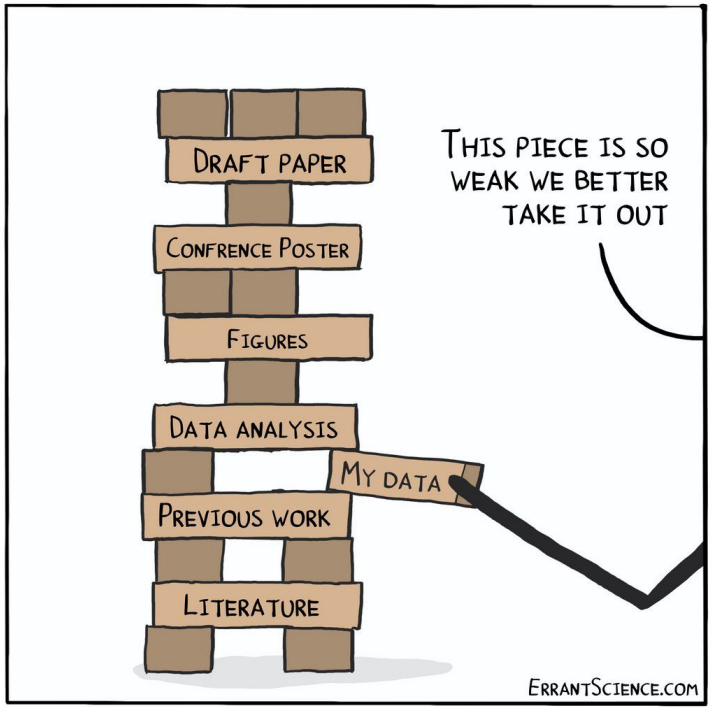
What are the barriers?
How can these be addressed?

Current Barriers & Challenges to Open and Transparent Digital Research



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- Data
- Standards
- Software
- Hardware
- Cost
- Time
- Trust
- People / Adoption

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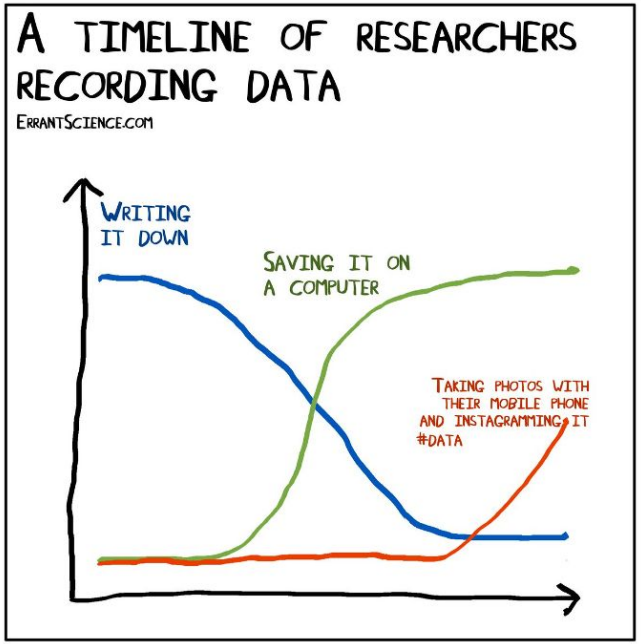
People/Adoption Barriers & Mitigations

Barriers

- **Resistance to change:** Hard to persuade people to change their processes
- **Group mentality:** Generally need to get entire group on board
- **Duplication of work:** Concerns about more work without seeing an obvious reward

Mitigations

- **Management:** A top down approach can make or break this
- **Demonstration:** Need to demonstrate how this will be of benefit
- **Start Afresh:** Implement this with a set of keen early adopters and or new starters for cooperation and to demonstrate success



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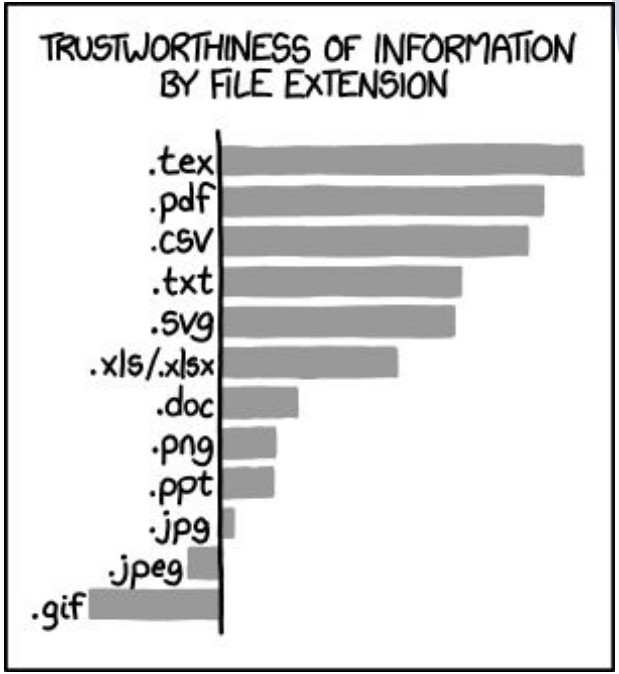
Data Barriers & Mitigations

Barriers

- **Un-FAIR Data:** Data frequently isn't findable, accessible, interoperable or re-useable
- **Metadata/Provenance:** Data often lacks context, its time consuming to capture metadata which leads to lack of provenance
- **Data Size:** Datasets are frequently too large to easily store/share

Mitigations

- **Education:** We need more training on how to how to make our data properly FAIR
- **Tooling & Guidelines:** We need better tools and guidelines to aid with capturing FAIR data and Metadata e.g. ELNs
- **Computing Resources:** We need access to centralised computing resources for storing/sharing data.



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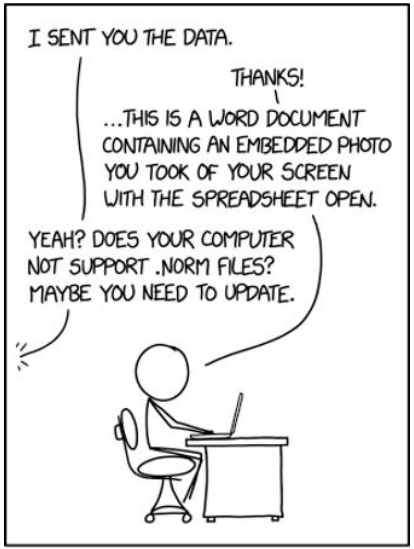
Standards Barriers & Mitigations



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Barriers

- **Too many standards:** There are both too many, and not enough standards
- **Proprietary Formats:** Industry software uses proprietary formats, causing vendor lock in and lack of compatibility
- **Lack of Interoperability:** There are many formats that don't work across multiple pieces of software

Mitigations

- **Open Source Formats:** Software should use open source formats that work across different tools and can be easily converted to/from
- **Format Conversion:** We need tools to convert between different data formats

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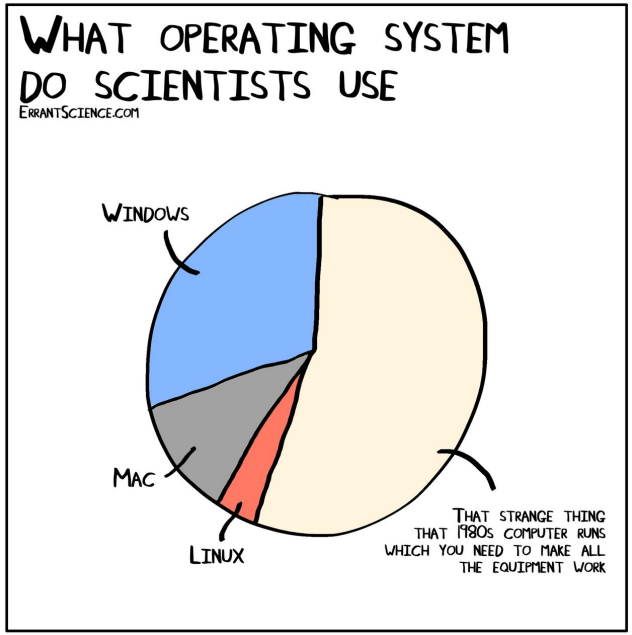
Software Barriers & Mitigations

Barriers

- **Software Choice Overload:** There are too many different pieces of software for digital research and data capture
- **Software Compatibility:** Software is frequently incompatible
- **Software Quality:** Users typically won't engage with software of poor quality

Mitigations

- **Resource Catalogues:** We need comprehensive information on the range of software available to make a suitable choice
- **Format Conversion:** We need tools to convert between different data formats so data can be used with different software
- **Software Design:** Involve actual software engineers, and train the scientists who make software in better practices



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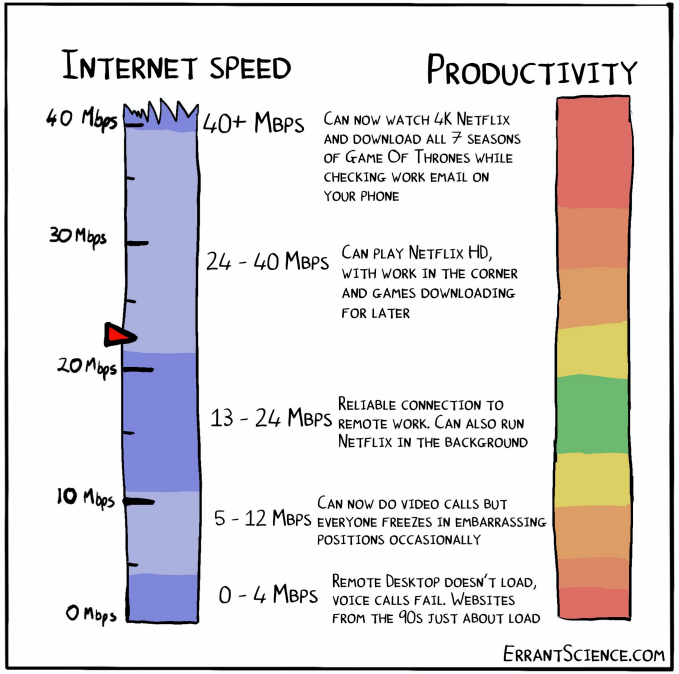
Hardware Barriers & Mitigations



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Barriers

- **Clunky Hardware:** Frequently available hardware won't run digital tools adequately, disengaging users completely
- **Legacy Equipment:** Too many laboratories use legacy equipment which requires legacy software and leads to producing outdated data formats
- **Hardware Cross Contamination:** Moving hardware in and out of the lab is dangerous and leads to contamination
- **Poor Internet Connection:** If there is lack of connectivity anything cloud/web based won't work

Mitigations

- **Invest in new Equipment:** We need to invest in new equipment to ensure smoother running of software and to reduce the requirement for legacy software/data
- **Dedicated Lab Hardware:** We need specific hardware for inside the lab, and separate hardware for outside the lab to reduce contamination
- **Internet Provisions:** Either have hardwired connections or boost your WIFI

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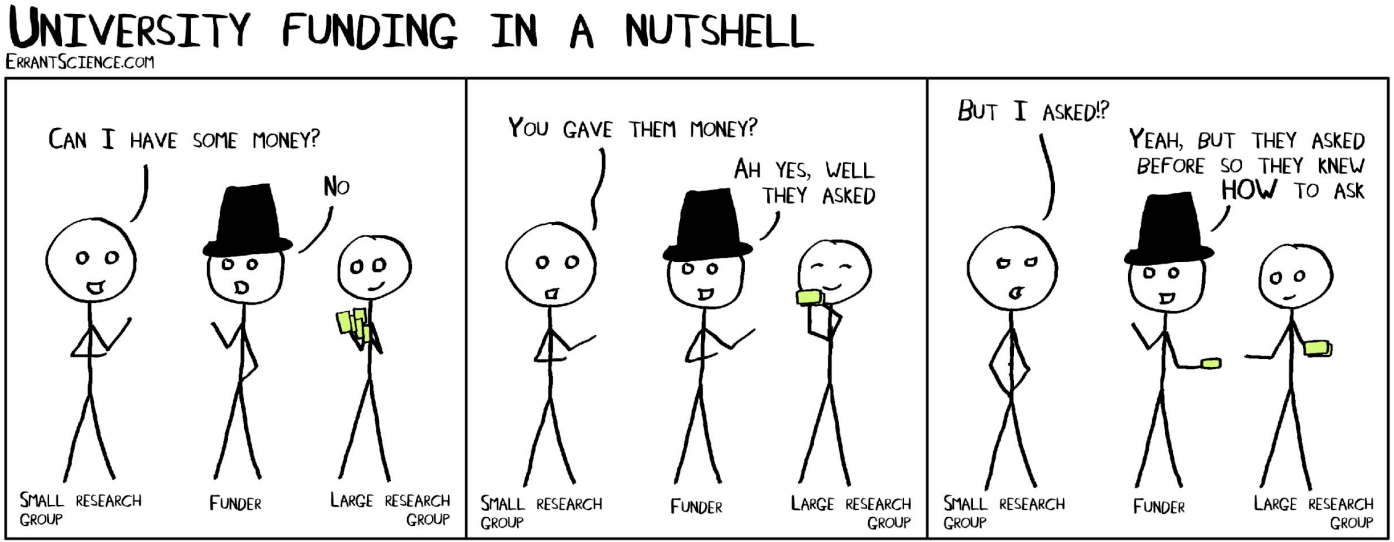
Cost Barriers

Barriers

- **Costs:** Funding, Research, Software, Hardware, Publishing

Mitigations

- **Embed in Funding Applications:** Extra costs to perform research data management properly with the appropriate expertise need to be embedded in applications
- **Investment:** Institutions need to invest in the appropriate hardware, software, education and addition staff e.g. Data Stewards to do this properly



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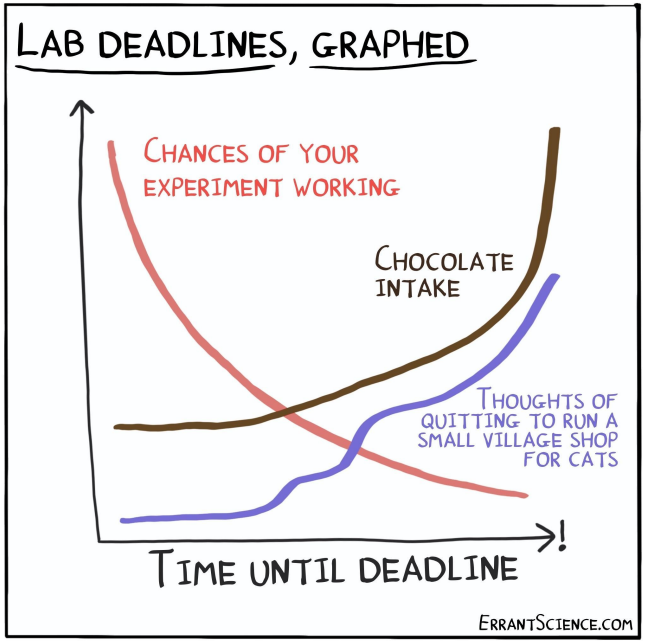
Time Barriers & Mitigations

Barriers

- **Learning:** Time taken to learn and use new systems
- **Do it Properly:** Doing research data management (RDM) properly is very time consuming
- **Current Systems:** without effective tools digitising data and capturing research in a transparent way is very time consuming

Mitigations

- **Start Early:** Make Data Management Plans and embed RDM into your entire project
- **Build in Time:** Projects need to formally build in time for research data management rather than seeing it as a “nice to have” or something that can be tacked on quickly at the end
- **Better Systems:** We need to develop better tools for capturing research and data



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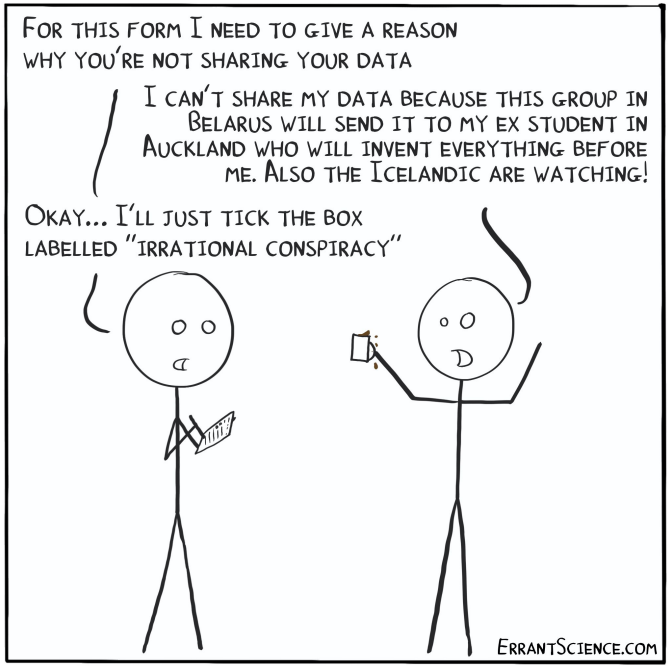
Trust Barriers & Mitigations



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Barriers

- **Cloud Storage:** Many researchers don't trust storing their data/research online due to concerns about:
  - **Data Privacy:** Sharing/Hacking
  - **Vendor Lockin:** Software using proprietary formats and lack of data exit strategy

Mitigations

- **Education:** We need more education about the genuine dangers of cloud based storage weighed up against paper / local storage
- **Storage Location:** There are options to store data "in the cloud" but with local servers e.g. MS Sharepoint and to have clever backup strategies to subvert hacking vulnerabilities

Planning ahead - key message

- There are still many barriers to overcome but the community is working towards solutions
- We need to remember to:
  - Start early and plan for your data, don't leave data management to the last minute
  - FAIR is a FOUR letter word, but has many nuances
  - Collaboration is key - this is a human AND technical endeavour
    We need to invest more time, money and resource into being FAIR

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These challenges are international

What international efforts are there?

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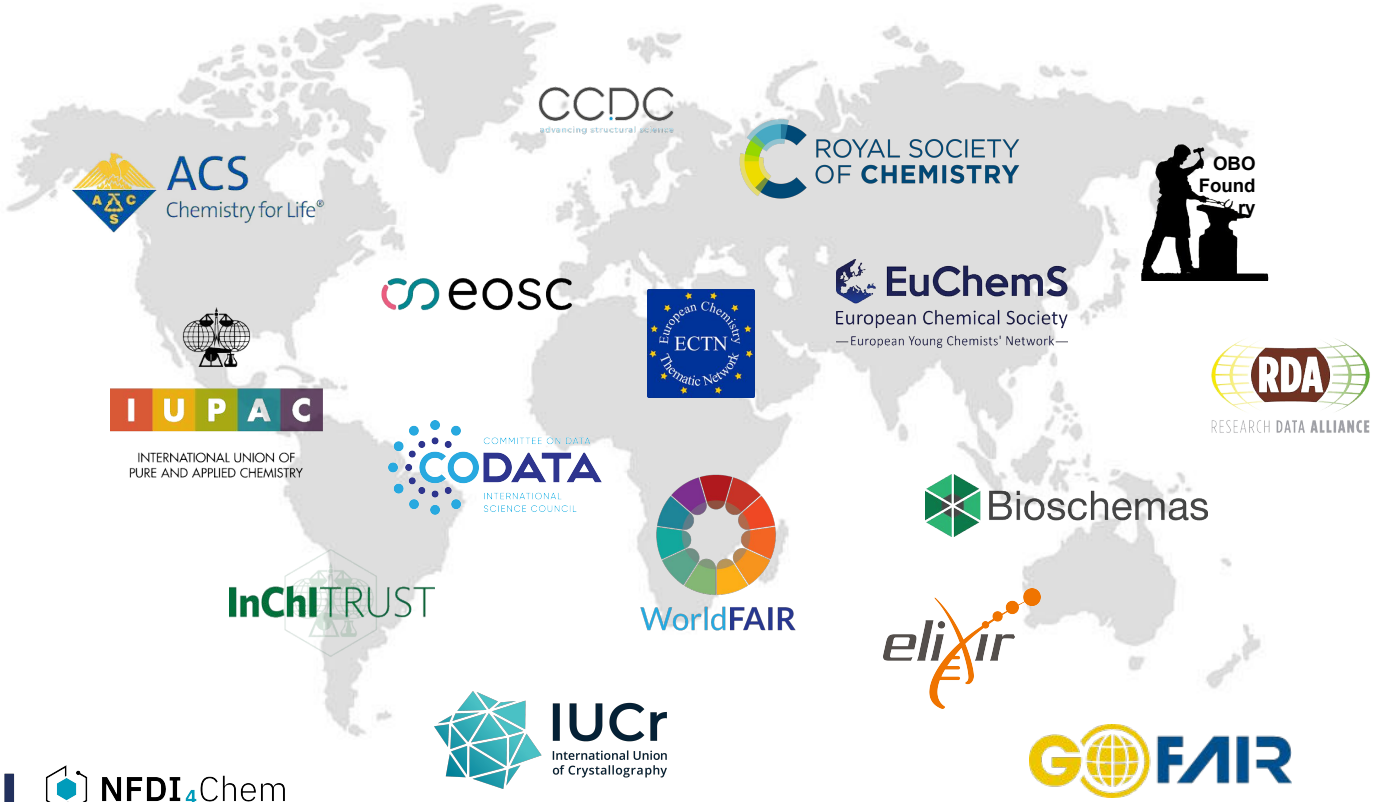
International Network of PSDI and NFDI4Chem



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IUPAC and Standards

- The International Union of Pure and Applied Chemistry (IUPAC) is the world authority on digital standards in chemistry; chemical nomenclature and terminology standardized methods for measurement; and on atomic weights
- IUPAC has been creating the common language of chemistry for more than a century.

IUPAC

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

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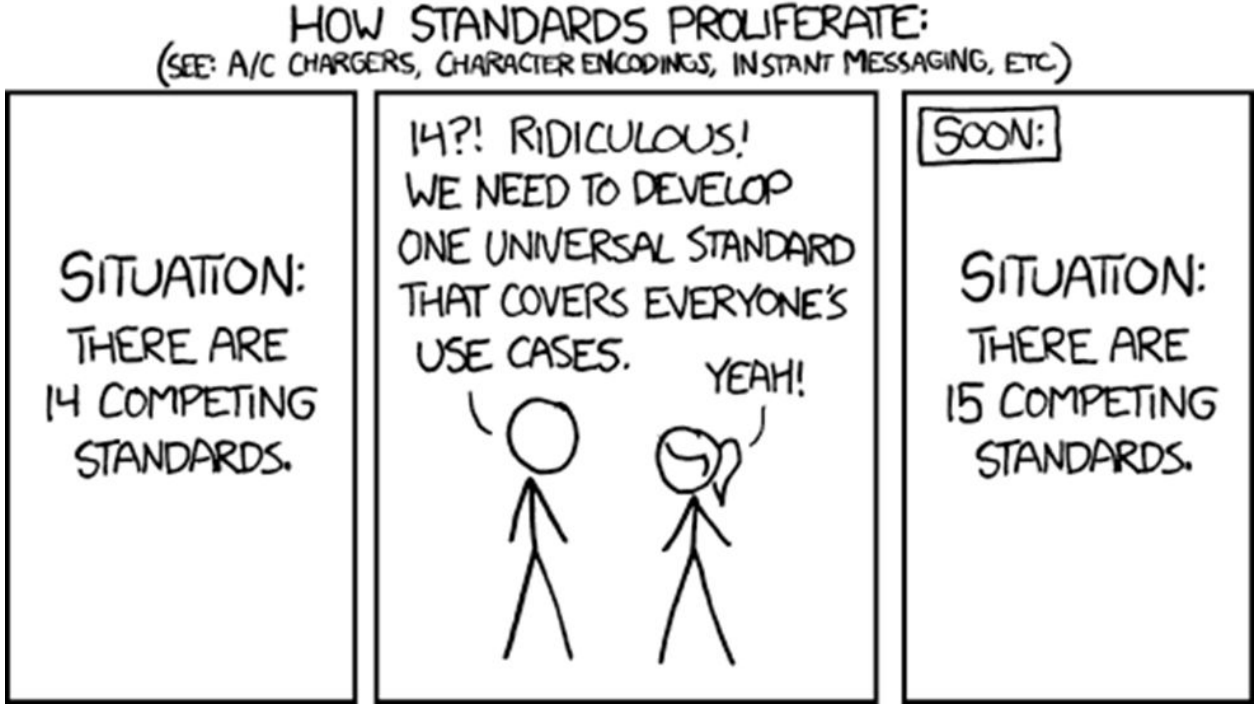
IUPAC and Standards

- Standards are important to advance the goals of FAIR data because:
  - **Uniformity and Clarity:** Ensure consistent chemical nomenclature and terminology.
  - **Seamless Data Exchange:** Facilitate smooth data sharing and collaboration.
  - **Reproducibility:** Enable accurate reproduction of experiments and results.
  - **Interoperability:** Promote data and tool interoperability.
  - **Global Collaboration:** Support effective collaboration worldwide.
  - **Enhanced Data Reusability:** Simplify data reuse, saving time and resources

Standards - the Challenge



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NFDI4Chem & PSDI Involvement in IUPAC

- Participation in IUPAC's involvement in World FAIR
  - FAIR Chemistry Cookbook
- InChI Trust
  - Development and maintenance of the InChI Standard
  - Promotion of InChI adoption in scientific communities
  - Collaboration with software developers for integration
- Committee on Publications and Cheminformatics Data Standards
  - Standard for FAIR Data Management of Spectroscopic Data (FAIRSpec)
  - Machine-Accessible Periodic Table
  - Development of guidelines for publication standards
- IUPAC Gold Book
  - Incorporation of new scientific terms and concepts, with regular updates

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IUPAC INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

NFDI4Chem's involvement in the InChI Trust

- Since 2020 involvement in the organometallics subgroup (until now, bonds to metals are disconnected)
- Since 2022: two InChI developers working at RWTH Aachen University on the next version of the InChI
- Since 2023: Sonja Herres-Pawlis was elected into the InChI Trust
- 2024: new InChI version v1.07 out as test version

  → the InChI has moved to GitHub, is now FAIR

  → free webdemo: https://iupac-inchi.github.io/InChI-Web-Demo/

- Organometallics/inorganics are programmed **now** into the InChI
- InChI in Action: technical workshop on 24th and 25th july in Aachen (contact Sonja Herres-Pawlis)

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InChITRUST
VolkswagenStiftung

IUPAC FAIR Cookbook (PSDI)

- Living community resource for managing digital chemical data effectively
- Enabling the move toward sharing and reusing data, code, metadata, etc.
- Step by step recipes for working with chemical data such as: using APIs to access chemical data or using chemical libraries in Python

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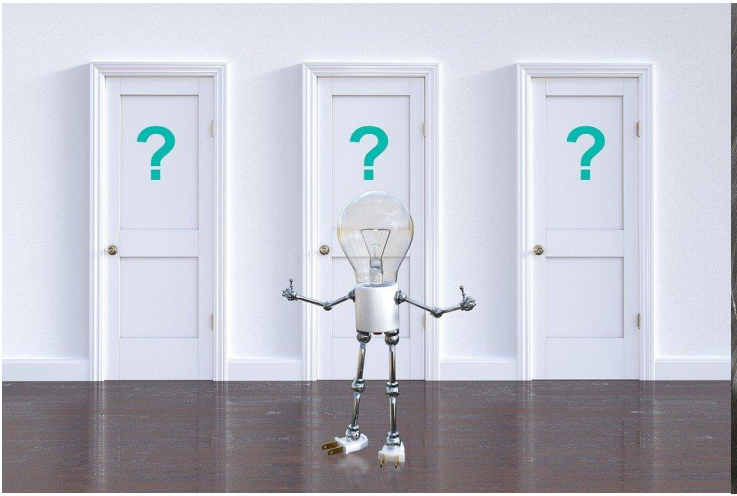
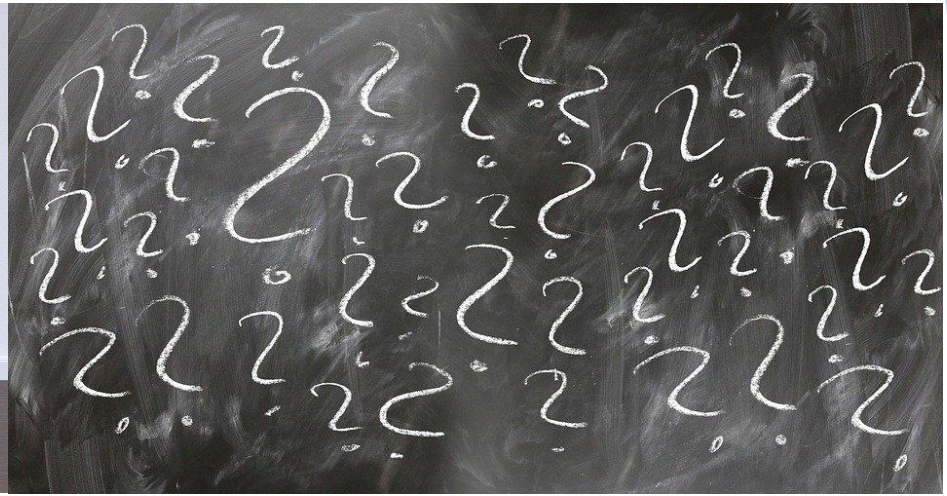
http://bit.ly/CookFAIR or
https://iupac.github.io/WFChemCookbook

Questions?





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