



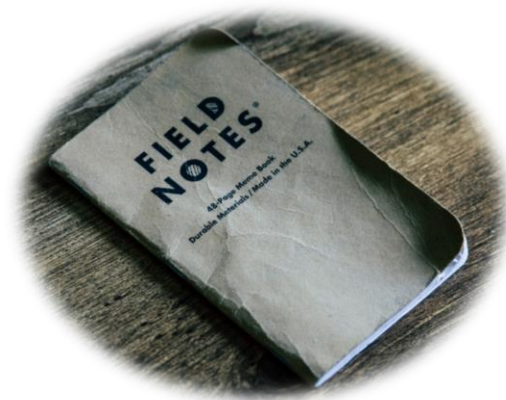
Record Keeping in the digital Age. Are you Ready?

Dr. Leo Betschart

Our Mission



Today's Journey



The Good Old Notebook



Most Basic Advantages of Electronic Record Keeping



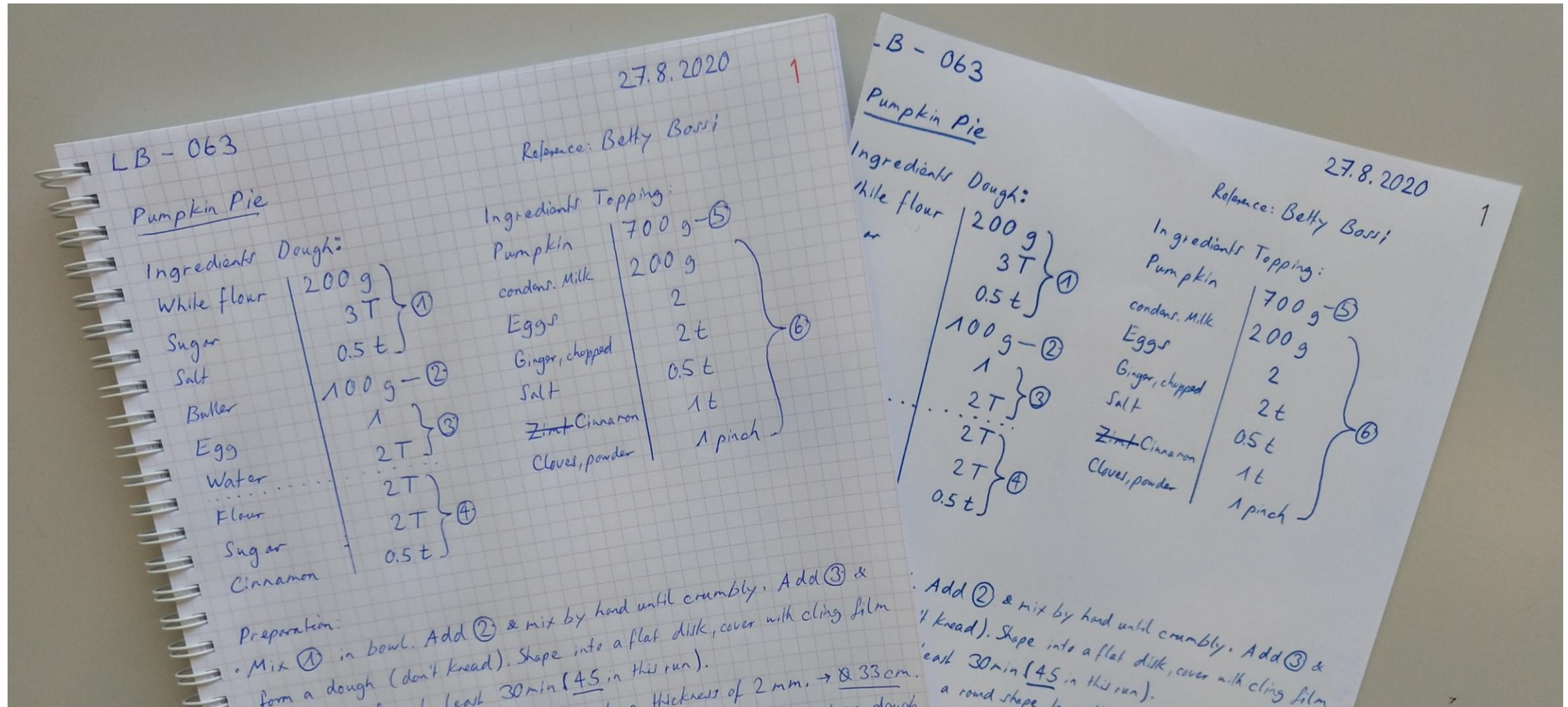
Your data is safely off premises.



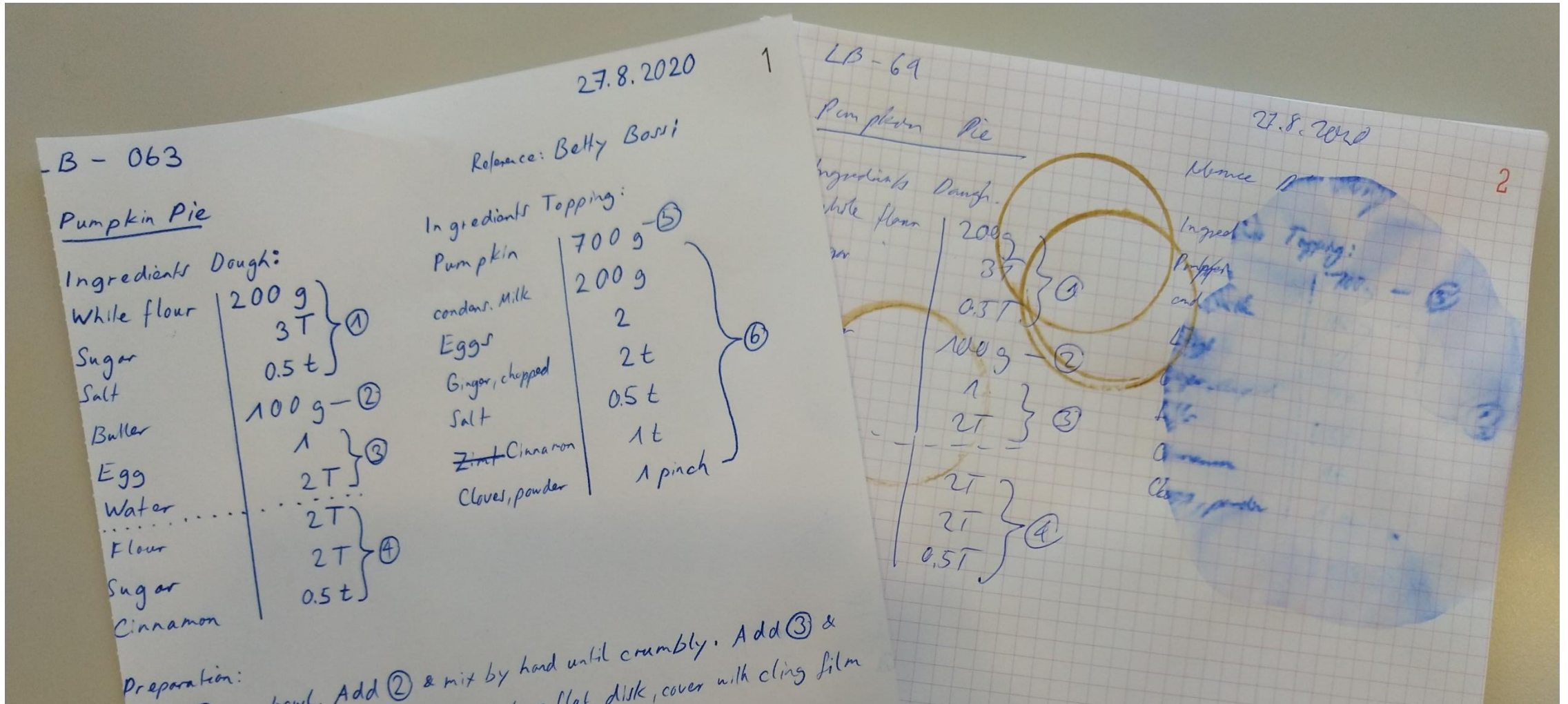
Your data is safely off premises.



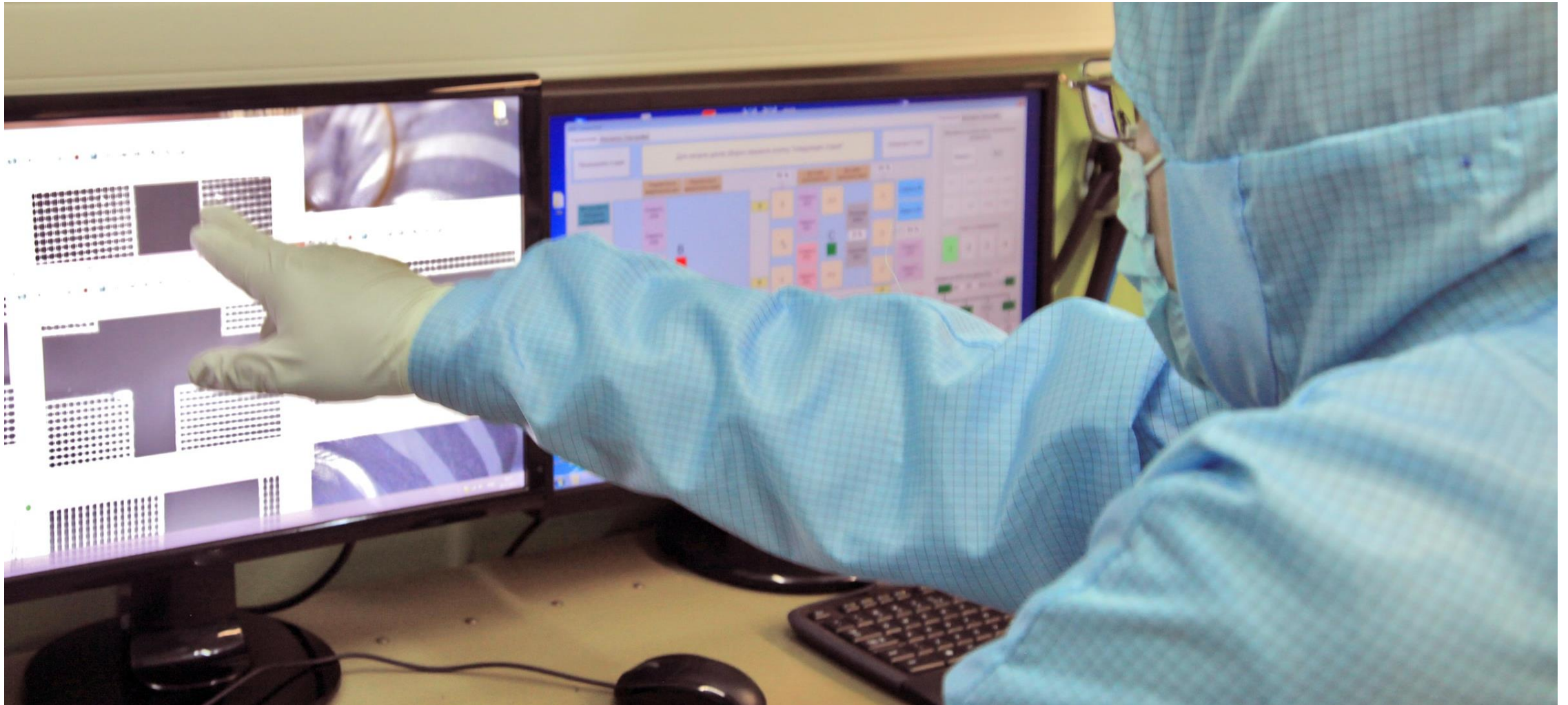
Data is backed up regularly and automatically.



Clean and legible records are created.



Easy to work in different or restricted labs (bio, radio, clean)



If that is all you need...



Importance of Data Integrity



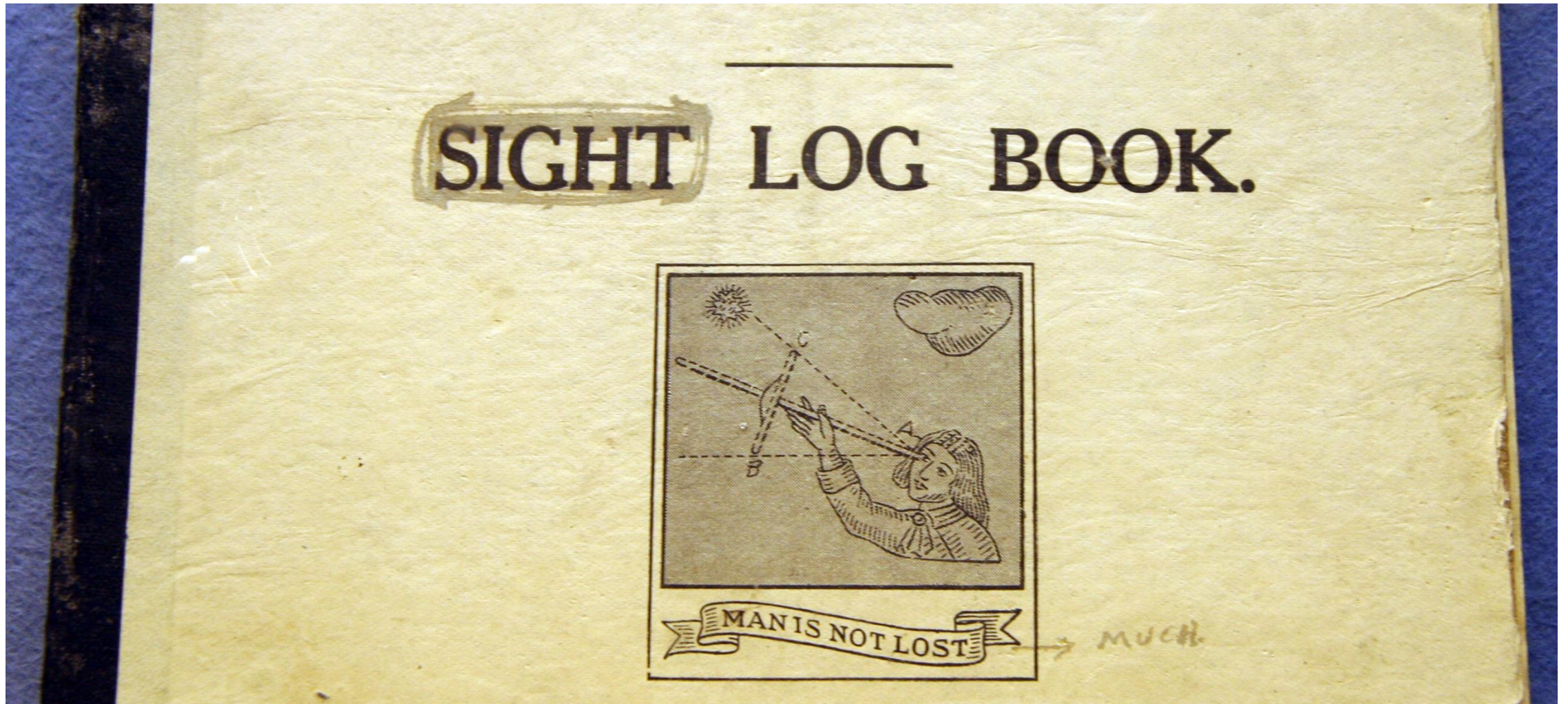
Access to data is easily controlled.



Granular control of reading/writing credentials.



Changes are documented and traced.



Disputes over Intellectual Property.



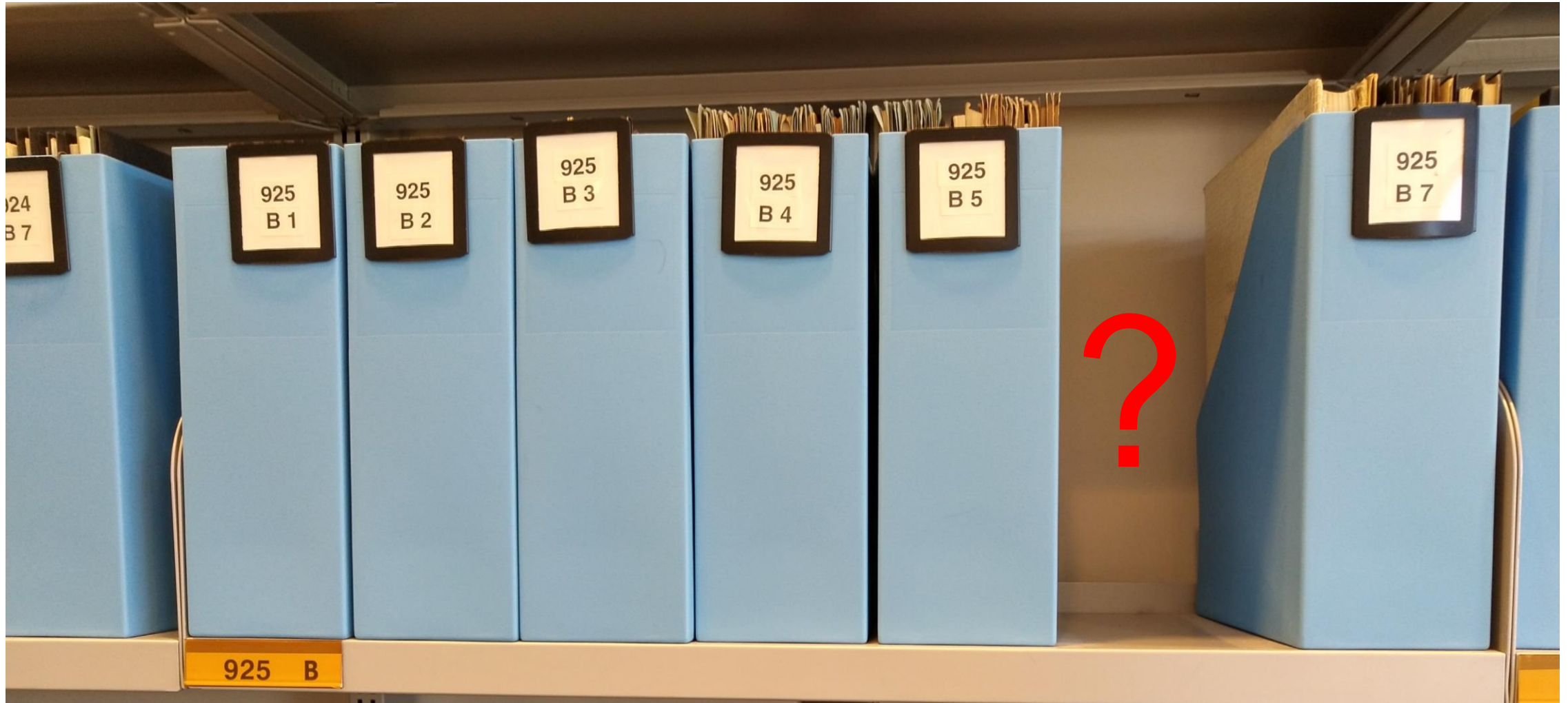
Automatic Timestamps



Data cannot be destroyed.



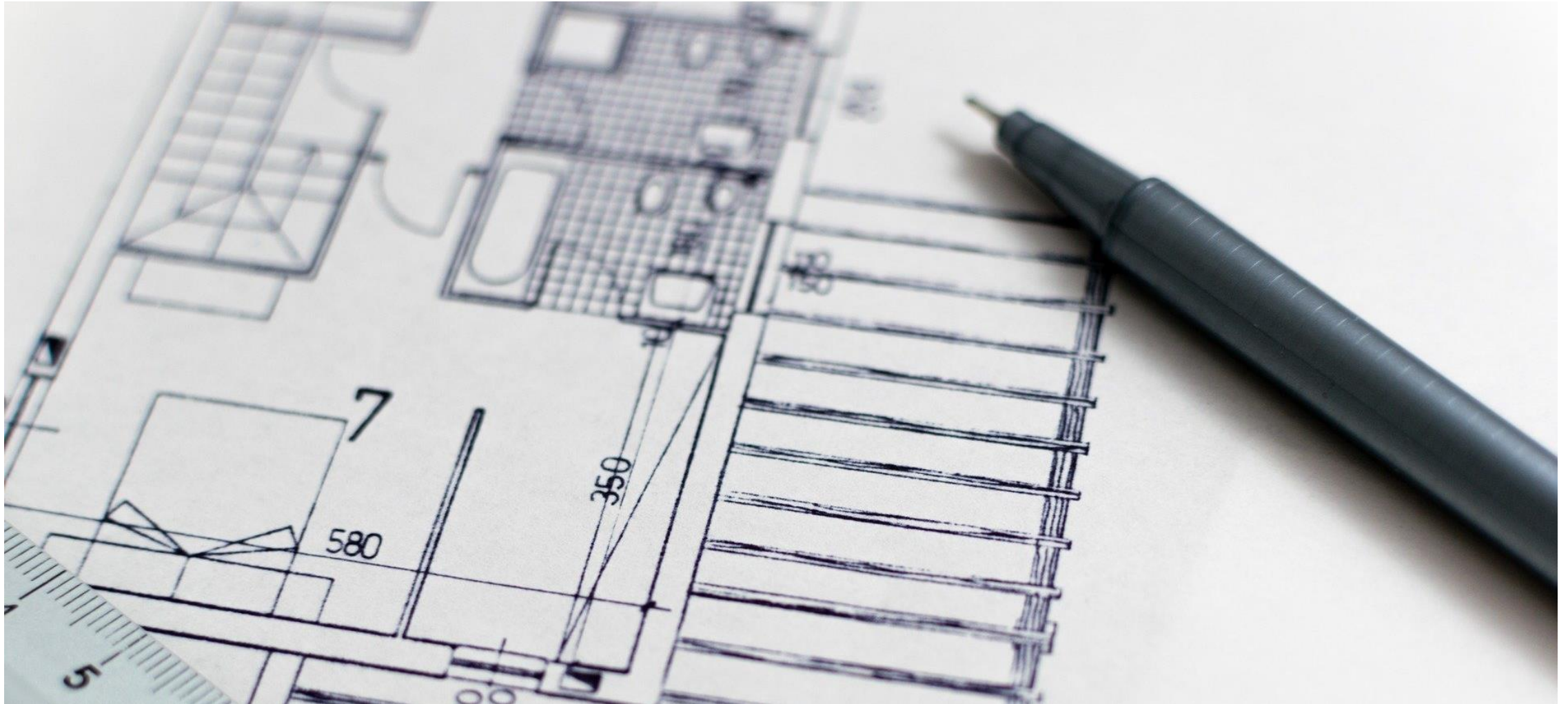
Data will not «disappear»



Perspective of a Supervisor



Fullfills requirements of Data Management Plan (DMP).



Creates Findable, Accessible, Interoperable, Reusable Data



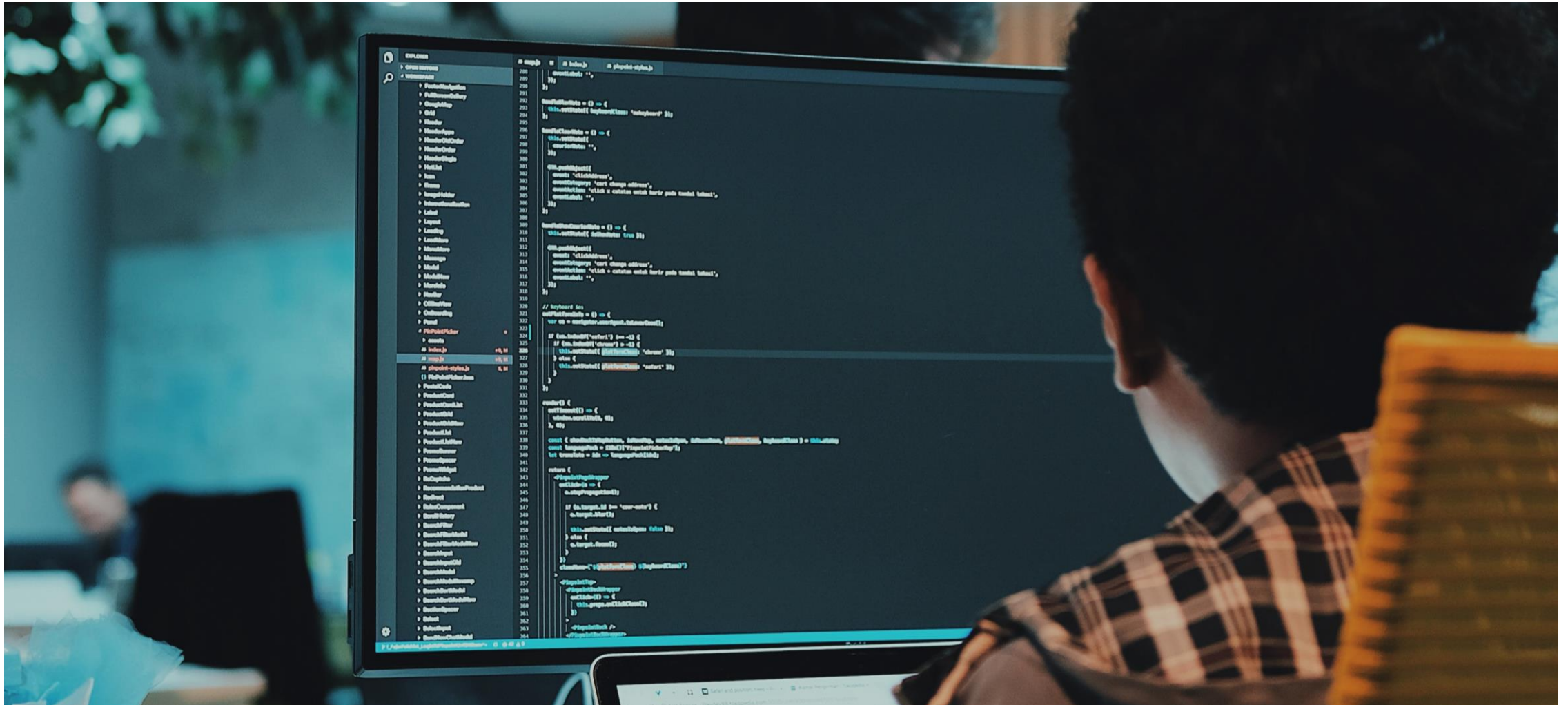
Standards for Record Keeping



Overview of Current Activities



Creation of Unique Datasets



Data can not be taken hostage.



Perspective of a Researcher



Writing becomes faster.

$IgG = \frac{22.63 \text{ MS}}{\text{mL}} \quad 880 \mu\text{L}$
 $BABE \sim 40 \text{ mM} \quad 100 \mu\text{L} \quad 4 \text{ mM}$
 $2\text{-IT} \quad 100 \text{ mM} \quad \frac{20 \mu\text{L}}{1000 \mu\text{L}} \quad 2 \text{ mM}$

$1.89 \mu\text{M}$
 $\text{in } 137 \mu\text{M } 90 \text{ mM}$
 Tris-HCl + Amine

pH was adjusted with $15 \mu\text{L}$ 2 M Tris-HCl + Amine, $\text{pH} = 9.01$
 Sample incubated at 37°C for 23 h , start $10:30$
 Sample removed from 37°C bath ~~at~~ $9:30$
 Purified by Penefsky column: 0.1 M NH_4OAc $\text{pH} = 6.93$
 Sephadex G 50-80 - 7 Penefskys a $155 \text{ mL} \rightarrow 1.085 \mu\text{L}$
 final $\text{pH} = 6.88$

Co57 Binding Assay

$100 \mu\text{L}$ NMEP_i -buffer $\text{pH} = 8.9$
 $20 \mu\text{L}$ Co57 1.02 mM
 $10 \mu\text{L}$ IgG - 2-IT - $BABE$

$\downarrow 40 \text{ min RT}$
 $15 \mu\text{L}$ 100 mM EDTA
 $\downarrow 20 \text{ min RT}$

} triplicate

The reaction was quenched with 20 ml H_2O and the solvents were removed under reduced pressure.

The residue was taken up in 20 ml water, the pH adjusted to 6.5 with 0.4 ml 2 M ammonium acetate, pH 9 , and purified by reversed-phase HPLC: solvent A, 0.1 M ammonium acetate pH 6.0 ; solvent B, methanol: $0\text{--}30 \text{ min}$ $25\text{--}40\%$ B, 12.5 ml/min , product 16 min ; and lyophilized to give 300 mg of the product biotinyl-LC-DOTA. Yield: 89% . $^1\text{H-NMR}$ (D_2O , pD 12): $1.2\text{--}3.3$ (m, 4H), 4.3 (m, 1H), 4.5 (m, 1H), 7.3 (m, 4H). FAB-MS: m/e calcd $\text{C}_{39}\text{H}_{60}\text{N}_4\text{O}_{11}\text{S}$ ($\text{M} + \text{H}^+$) 849.4 , found: 849.6 .

2.8.8. Biotinyl-LC-DOTA metal-binding assays
 Biotinyl-LC-DOTA binding assays were performed as follows: biotinyl-LC-DOTA was dissolved in 2 M ammonium acetate, pH 9 , giving a final concentration of 18.8 mM . Equal amounts of biotinyl-LC-DOTA, 27.5 mM $^{57}\text{Co}/\text{Co}$ solution and 2 M ammonium acetate, pH 9 , were mixed and incubated for 40 min . Assays were carried out as described [34] by TLC.

2.8.9. Biotinyl-LC-DOTA avidin binding assays
 These were carried out with 1.32 mM biotinyl-LC-DOTA (0.1 M ammonium acetate, pH 7.3) stock solution.
 Avidin solution: 10 mg avidin (egg white, lyophilized) was dissolved in 1 ml 0.1 M tetramethylammonium acetate, pH 7.9 , giving a concentration of 0.15 mM . Avidin concentration was estimated by measuring the UV absorption at 280 nm . $E_{280}^{1\%} = 12.5$ was taken from [39].
 Streptavidin solution: 1.0 mg of streptavidin peroxidase conjugate, lyophilized, from 0.1 M phosphate buffered saline, pH 7.5 , was reconstituted in 0.4 ml H_2O , giving a concentration of 25 mM . $E_{280}^{1\%}$ was determined as 15.8 ± 0.2 .

2.8.9.1. Binding of biotinyl-LC-DOTA to avidin (postcomplex labeling procedure). 0.8 ml of a 0.15 mM avidin solution (pH 7.9) was added to 0.4 ml of a 1.32 mM biotinyl-LC-DOTA solution (pH 7.3). The pH was adjusted to 8.9 .

2.8.9.2. Binding of biotinyl-LC-DOTA to streptavidin (precomplex labeling procedure). $10 \mu\text{L}$ of a 27.5 mM $\text{Co}/^{57}\text{Co}$ solution was added to $100 \mu\text{L}$ of a 1.32 mM biotinyl-LC-DOTA solution. After incubation for 1 h , the solution was added to $300 \mu\text{L}$ of the streptavidin solution. Aliquots of this mixture were incubated (i) at 37°C and (ii) at room temperature for 2 h .
 Excess $\text{Co}/^{57}\text{Co}$ was removed by adding EDTA to the incubated solution prior to purification by gel-filtration centrifugation, described above. The relative chelate to streptavidin ratio was determined from UV absorbance and radioactivity of the isolated product.

3. Results and discussion
3.1. Synthesis of the biotinylated-chelate-conjugates
 The avidin-biotin system is widely used for *in vitro* and *in vivo* applications, in immunohistochemistry, ELISA and molecular biology [40,41]. Avidins are proteins that bind biotin with high affinity and specificity [42]. They can bind up to four molecules of biotin and the dissociation constant of the avidin-biotin complex is in the order of 10^{-15} M [43] so that binding can be considered an irreversible process.
 The fact that the binding sites for biotin occur in pairs fairly close

Project Management



Facilitates Sharing and Teamwork



Collective Memory



Content is Organized and Efficiently Searchable



No Need to Reinvent the Wheel



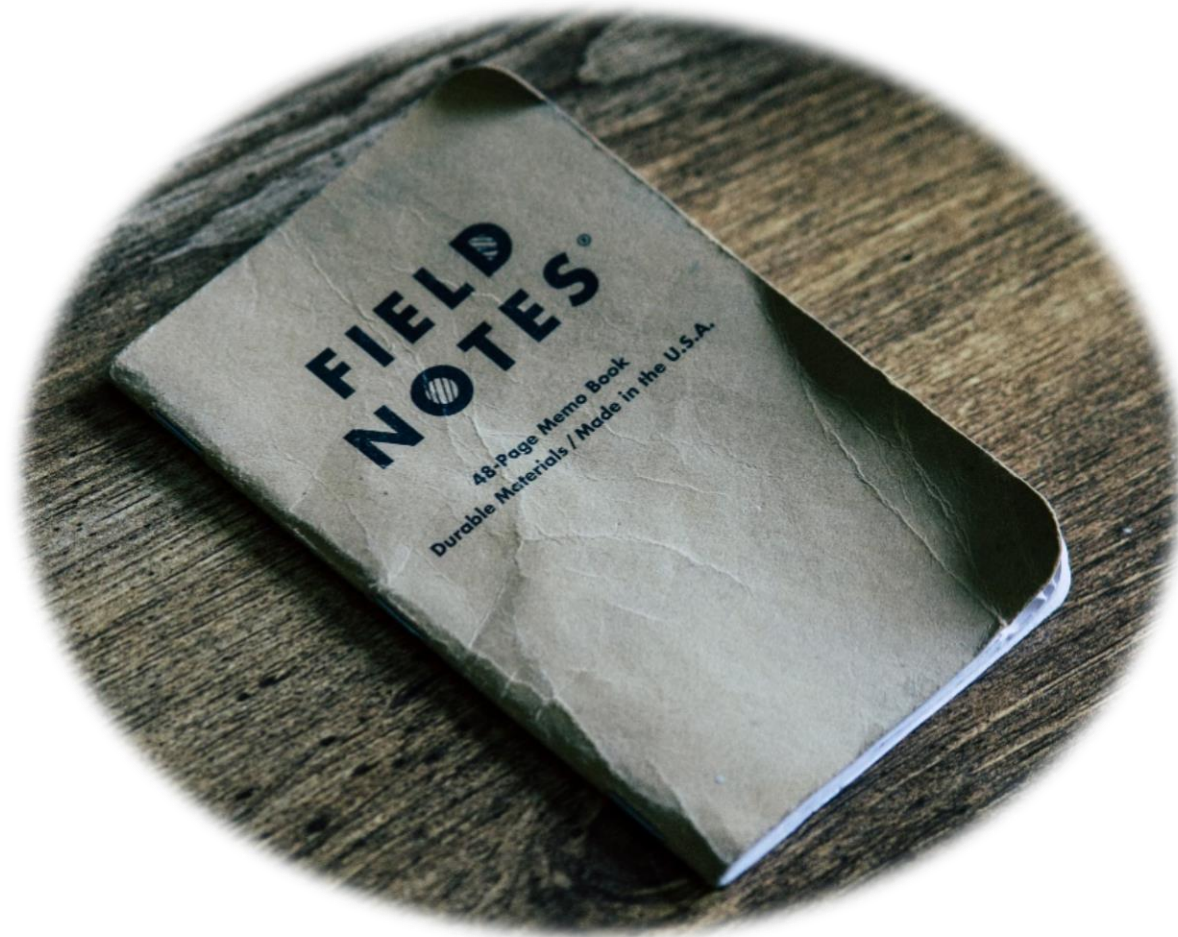
Remember failures of the past!



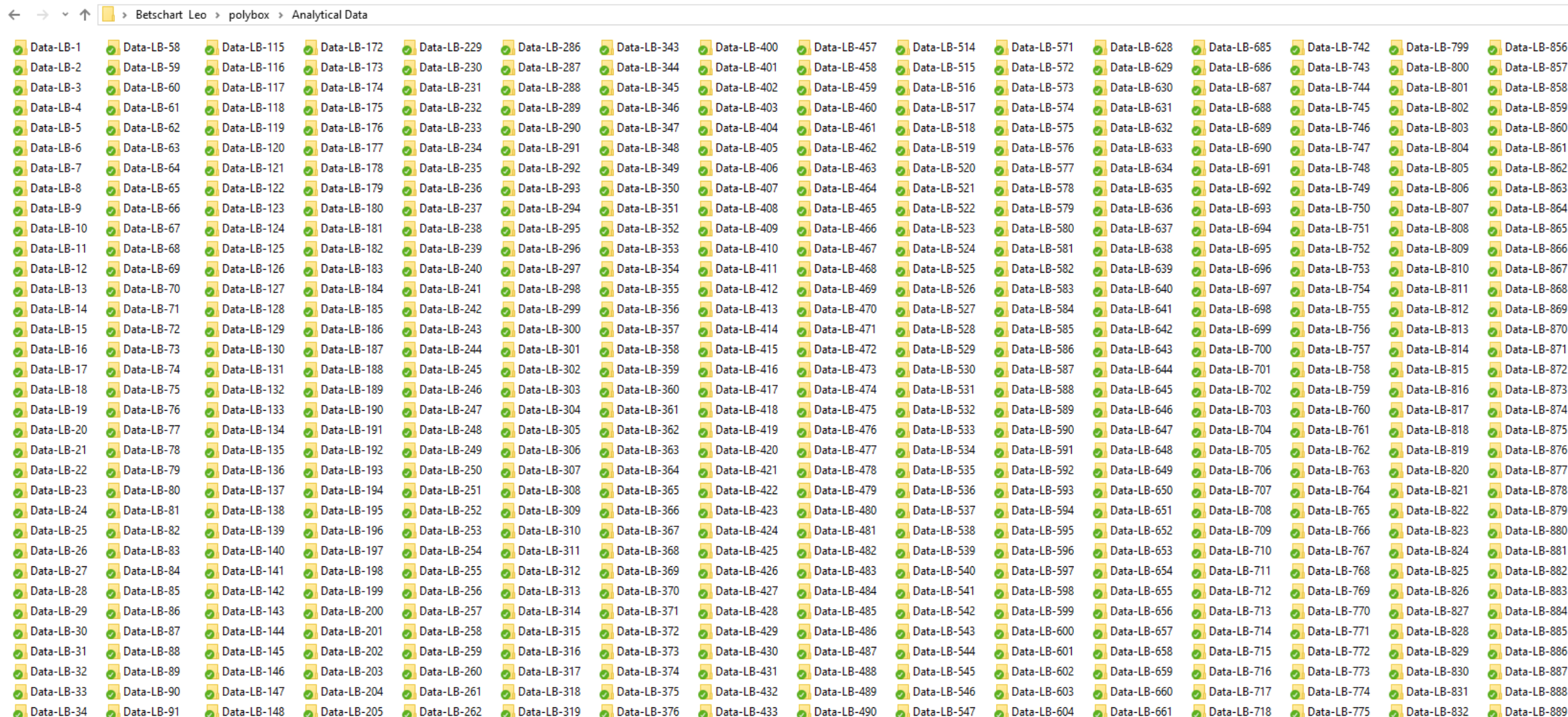
How many needles were there?



More than paper: How a researchers life might become easier.



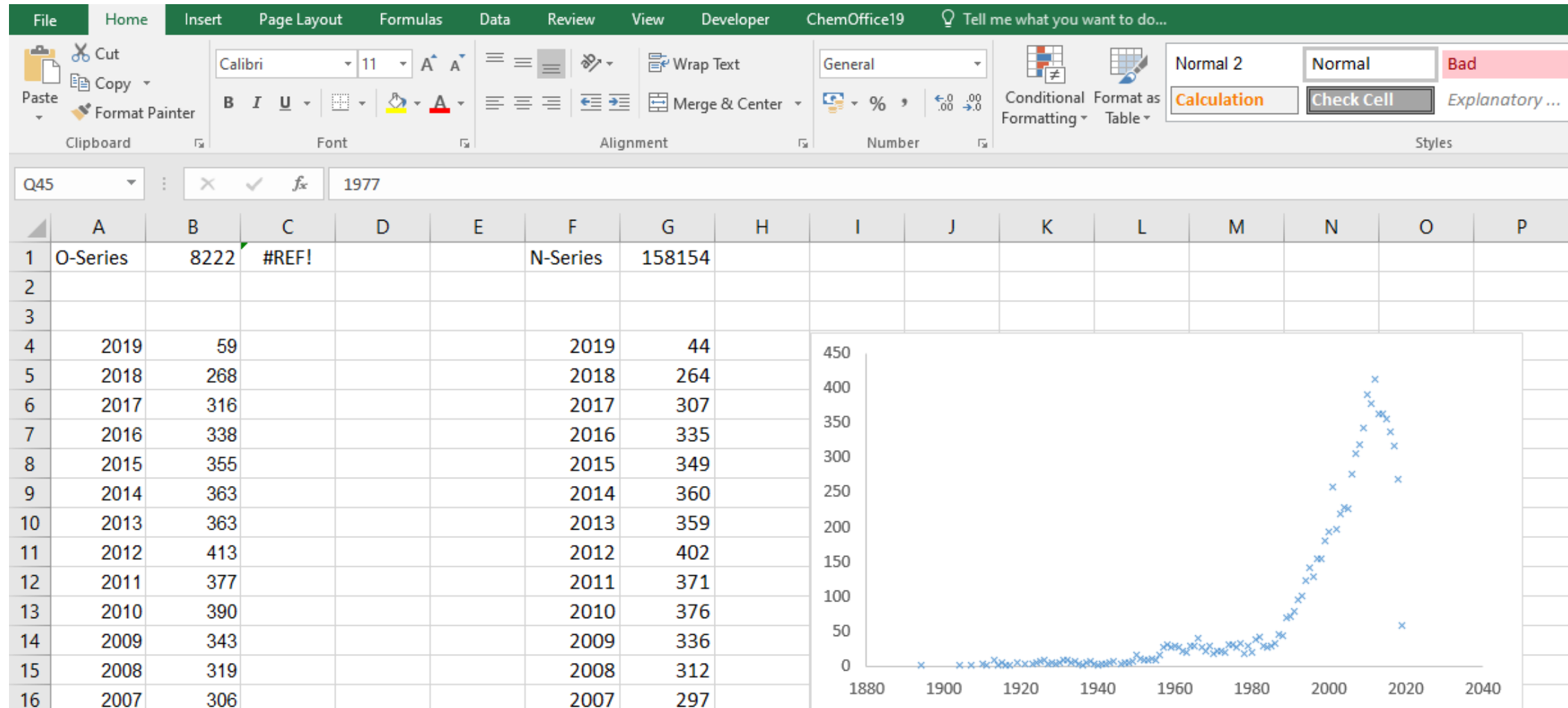
Store data together with lab notes.



Direct Import of Data from Devices



Spreadsheets



Baking a Smaller Pie



Templated Calculations

Anzahl Personen

200 g Ruchmehl
3 EL Zucker
0.25 TL Salz
100 g Butter, in Stücken, kalt
1 Ei, verklopft
2 EL Wasser

2 EL Mehl
2 EL Zucker
0.25 TL Zimt

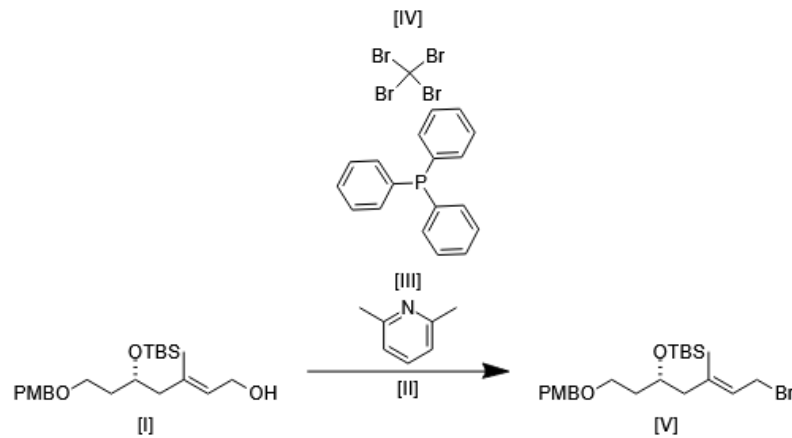
Anzahl Personen

75 g Ruchmehl
1.13 EL Zucker
0.09 TL Salz
37.5 g Butter, in Stücken, kalt
0.38 Ei, verklopft
0.75 EL Wasser

0.75 EL Mehl
0.75 EL Zucker
0.09 TL Zimt

Chemical Drawing and Calculation (1/4)

ChemDraw Document >



Quick

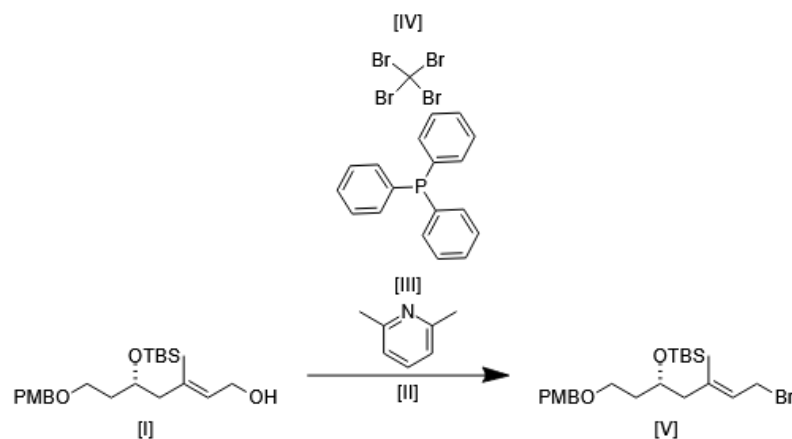
Reactants

Rxn ID
I
II
III
IV



Chemical Drawing and Calculation (2/4)

ChemDraw Document >



Quick

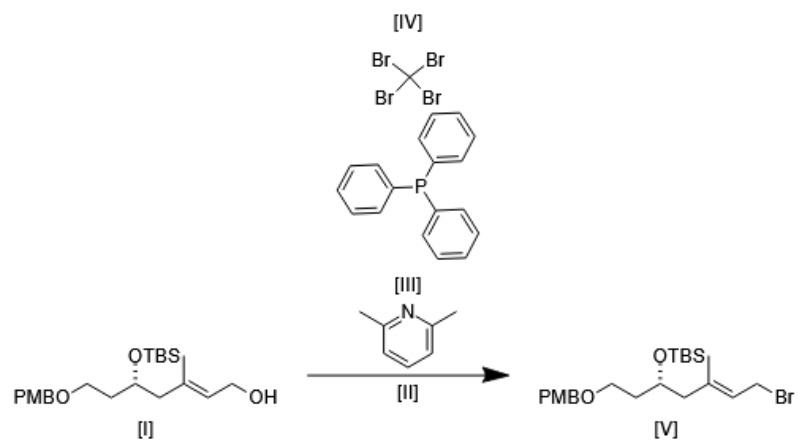
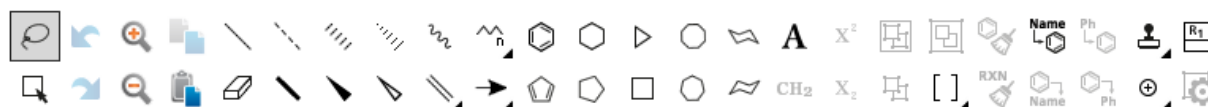
Reactants

	Rxn ID
	I
	II
	III
	IV

Eq	Sample Mass
1	2.6 g
1.6	1.1 g
2.2	3.8 g
2.2	4.8 g

Chemical Drawing and Calculation (3/4)

ChemDraw Document >



Quick

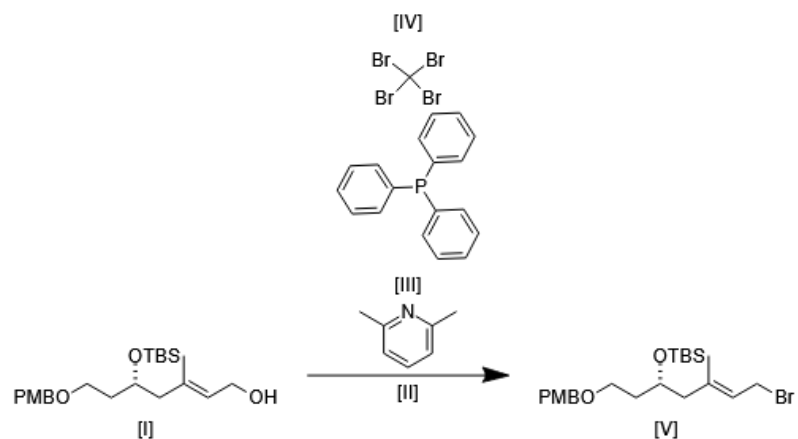
Reactants

⚙️	Rxn ID
▶	I
▶	II
▶	III
▶	IV

Eq	Sample Mass	Moles
1	2.6 g	6.6 mmol
1.6	1.1 g	11 mmol
2.2	3.8 g	14 mmol
2.2	4.8 g	14 mmol

Chemical Drawing and Calculation (4/4)

ChemDraw Document >



Quick

Reactants

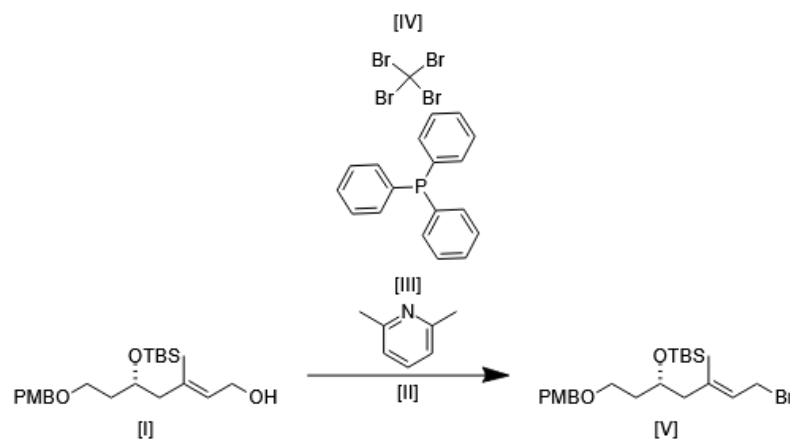
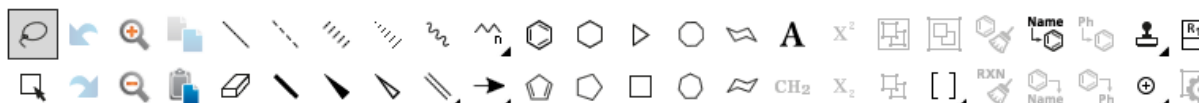
Rxn ID
I
II
III
IV

MF	FM
$C_{22}H_{38}O_4Si$	394.63
C_7H_9N	107.16
$C_{18}H_{15}P$	262.29
CB_r_4	331.63

Eq	Sample Mass	Moles
1	2.6 g	6.6 mmol
1.6	1.1 g	11 mmol
2.2	3.8 g	14 mmol
2.2	4.8 g	14 mmol

Data Retrieval from External Sources

ChemDraw Document >



Quick Add

Reactants

Rxn ID	Reactant	MF	FM
I	(R,E)-5-((tert-butylidimethylsilyl)oxy)-7-((4-methoxybenzyl)oxy)-3 ...	C ₂₂ H ₃₈ O ₄ Si	394.63
II	2,6-lutidine	C ₇ H ₉ N	107.16
III	triphenylphosphine	C ₁₈ H ₁₅ P	262.29
IV	CBr ₄	CBr ₄	331.63

Eq	Sample Mass	Moles
1	2.6 g	6.6 mmol
1.6	1.1 g	11 mmol
2.2	3.8 g	14 mmol
2.2	4.8 g	14 mmol

Vol	d
1.2 mL	0.92 g/ml

Reproducible Data Processing (R or Python)



```
In [1]: # Import required library
import pandas as pd
```

After the import command, we now have access to a large number of pre-built classes and functions. This assumes the library is installed; in our lab environment all the necessary libraries are installed. One way pandas allows you to work with data is a dataframe. Let's go through the process to go from a comma separated values (.csv) file to a dataframe. This variable `csv_path` stores the path of the .csv, that is used as an argument to the `read_csv` function. The result is stored in the object `df`, this is a common short form used for a variable referring to a Pandas dataframe.

```
In [2]: # Read data from CSV file

csv_path = 'https://s3-api.us-geo.objectstorage.softlayer.net/cf-courses-data/CognitiveClass/PY0101EN/Chapter%204/Datasets/Top50.csv'
df = pd.read_csv(csv_path)
```

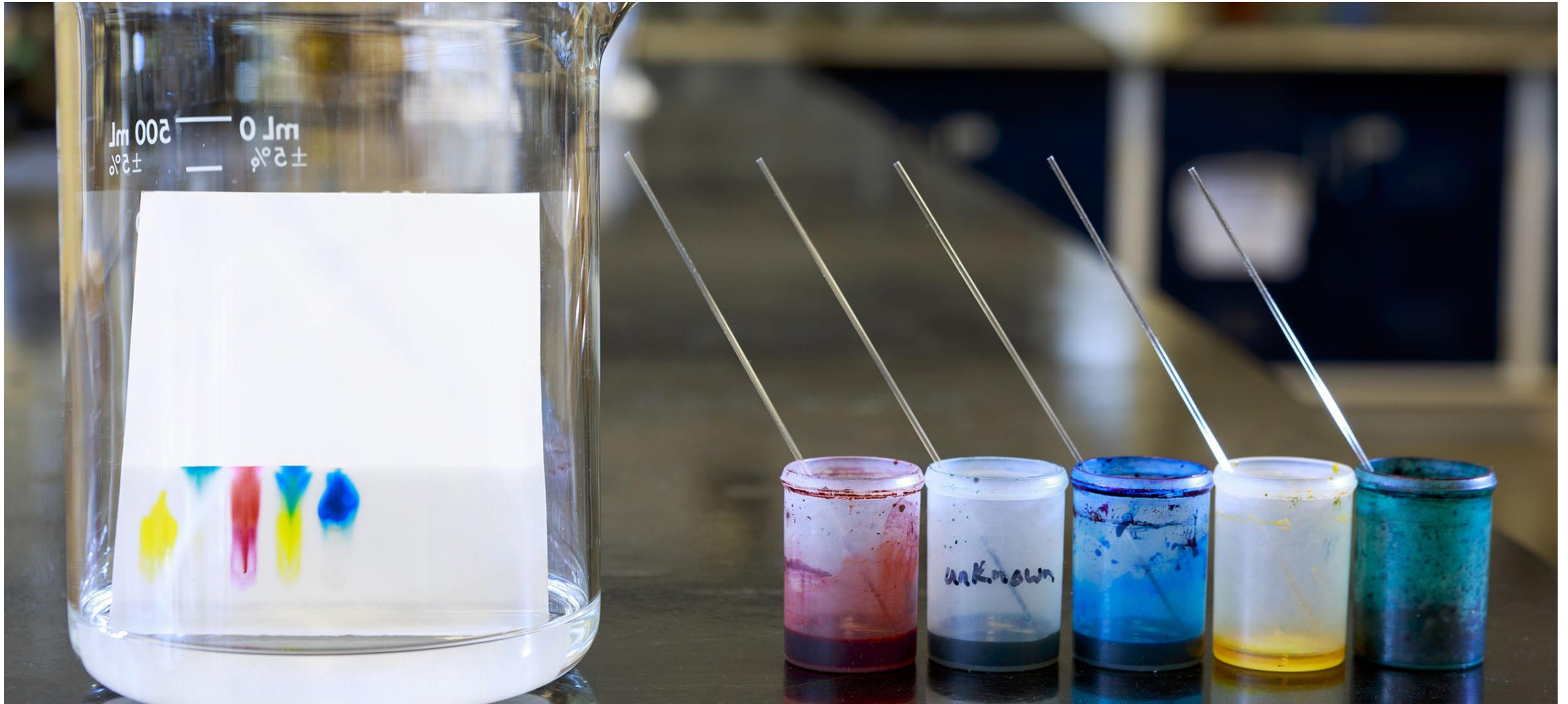
We can use the method `head()` to examine the first five rows of a dataframe:

```
In [3]: # Print first five rows of the dataframe
df.head()
```

Out[3]:

	Artist	Album	Released	Length	Genre	Music Recording Sales (millions)	Claimed Sales (millions)	Released.1	Soundtrack	Rating
0	Michael Jackson	Thriller	1982	0:42:19	pop, rock, R&B	46.0	65	30-Nov-82	NaN	10.0
1	AC/DC	Back in Black	1980	0:42:11	hard rock	26.1	50	25-Jul-80	NaN	9.5
2	Pink Floyd	The Dark Side of the Moon	1973	0:42:49	progressive rock	24.2	45	01-Mar-73	NaN	9.0
3	Whitney Houston	The Bodyguard	1992	0:57:44	R&B, soul, pop	27.4	44	17-Nov-92	Y	8.5
4	Meat Loaf	Bat Out of Hell	1977	0:46:33	hard rock, progressive rock	20.6	43	21-Oct-77	NaN	8.0

Easy Upload of Photo or Video Data



Assign Unique Identifiers for Experiments

10.1002/anie.201904584

0000-0003-2612-6616

58-08-2



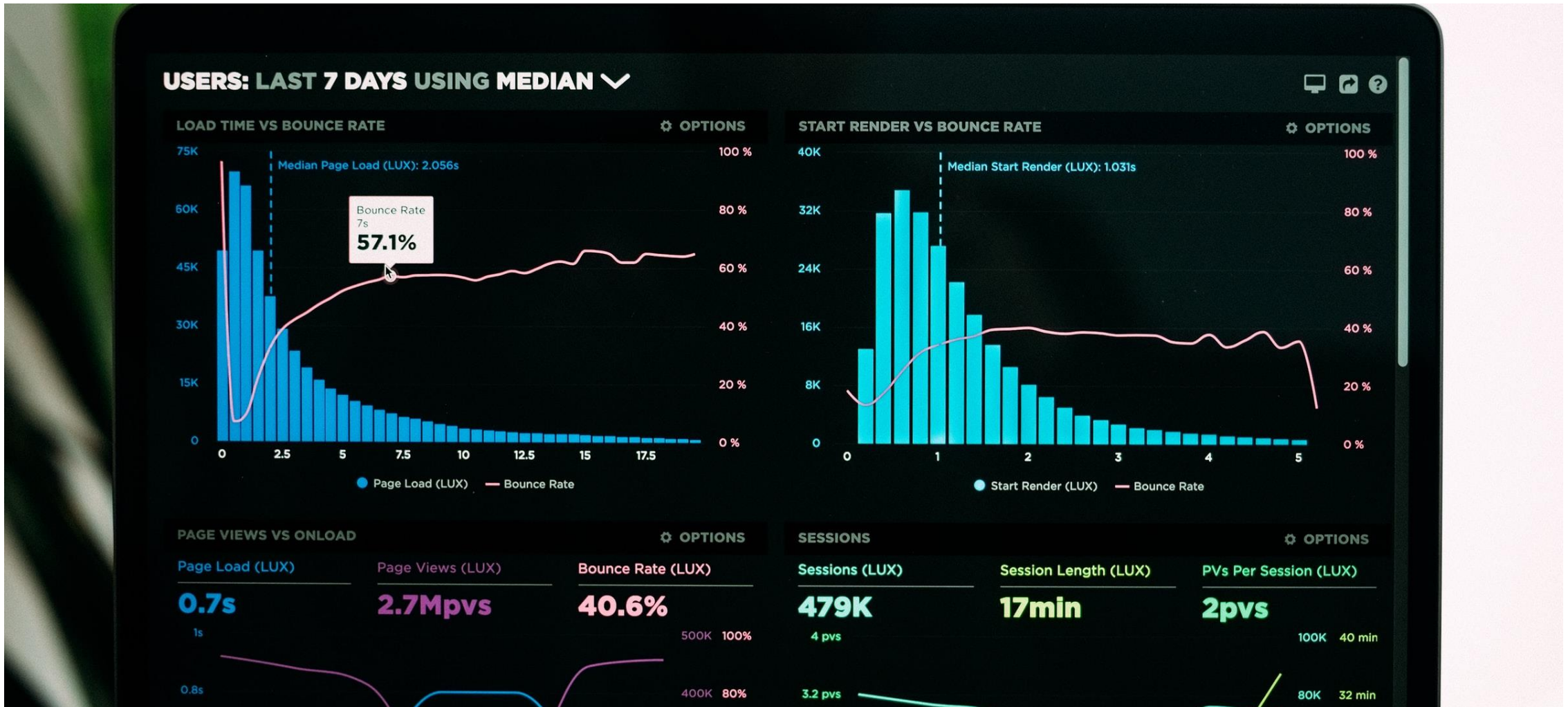
0362-4331

978-0439708180

Linked and Sequential Experiments



Planning Tools



Why so slow?



Cost is the most defining factor.



Price comparison



- CHF 8
- 50 flimsy pages
- Carbon copy



- CHF 6
- 161 sturdy pages

How much wasted time do you need to pay for an ELN licence?

Based on SNF stipends

Monthly Salary

Daily Salary (Ø 22 per month)

Days to reach CHF 450

How much wasted time do you need to pay for an ELN licence?

Based on SNF stipends

	PhD Student
Monthly Salary	3920
Daily Salary (Ø 22 per month)	178
Days to reach CHF 450	2.5

How much wasted time do you need to pay for an ELN licence?

Based on SNF stipends

	PhD Student	Postdoc
Monthly Salary	3920	7380
Daily Salary (Ø 22 per month)	178	335
Days to reach CHF 450	2.5	1.3

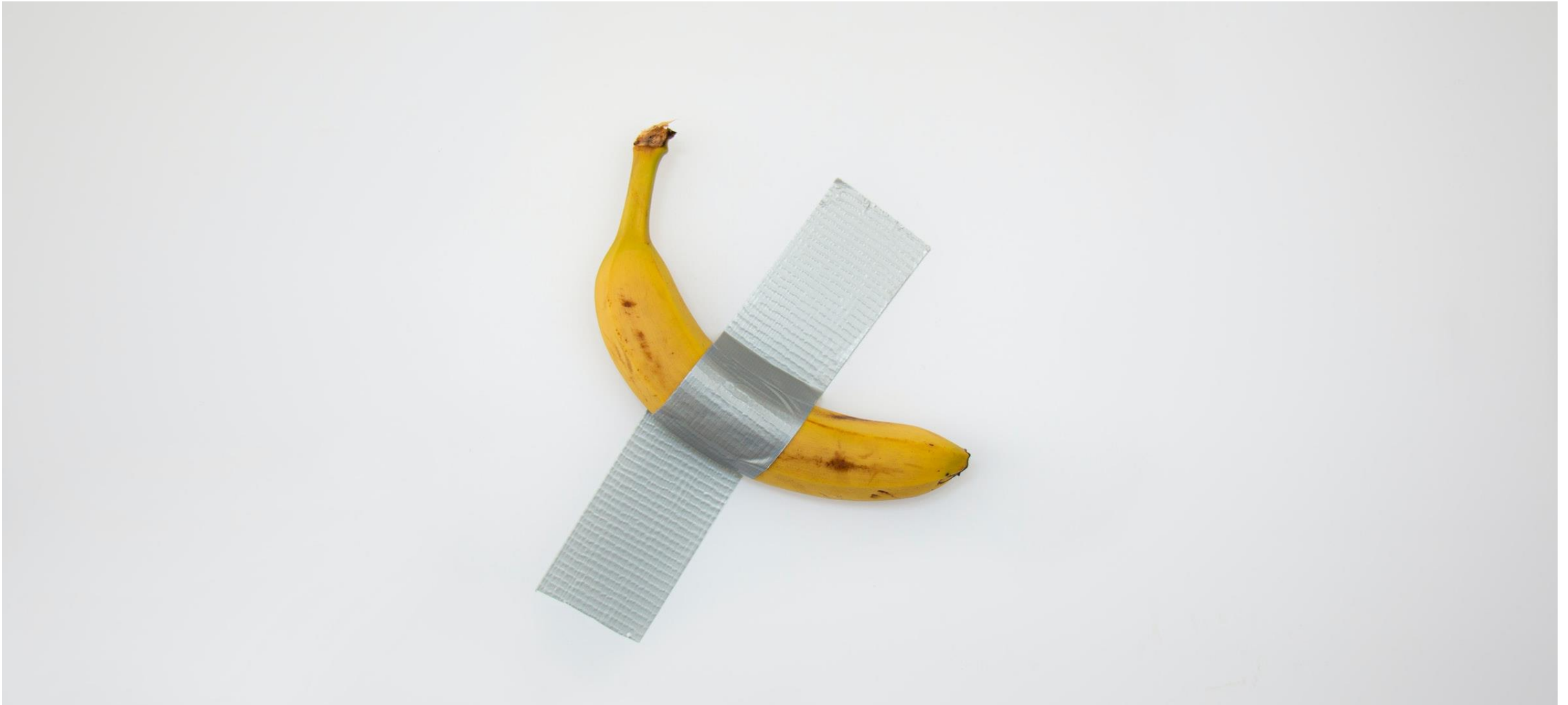
Nobody wants to be the first.



Students coming and going.



Petty Criteria



Bad Demos



Must-haves



The privacy paradox: Is data safe in the clouds?



What should you take home?



A tool and not a cure.



Out-of the box vs. customizable



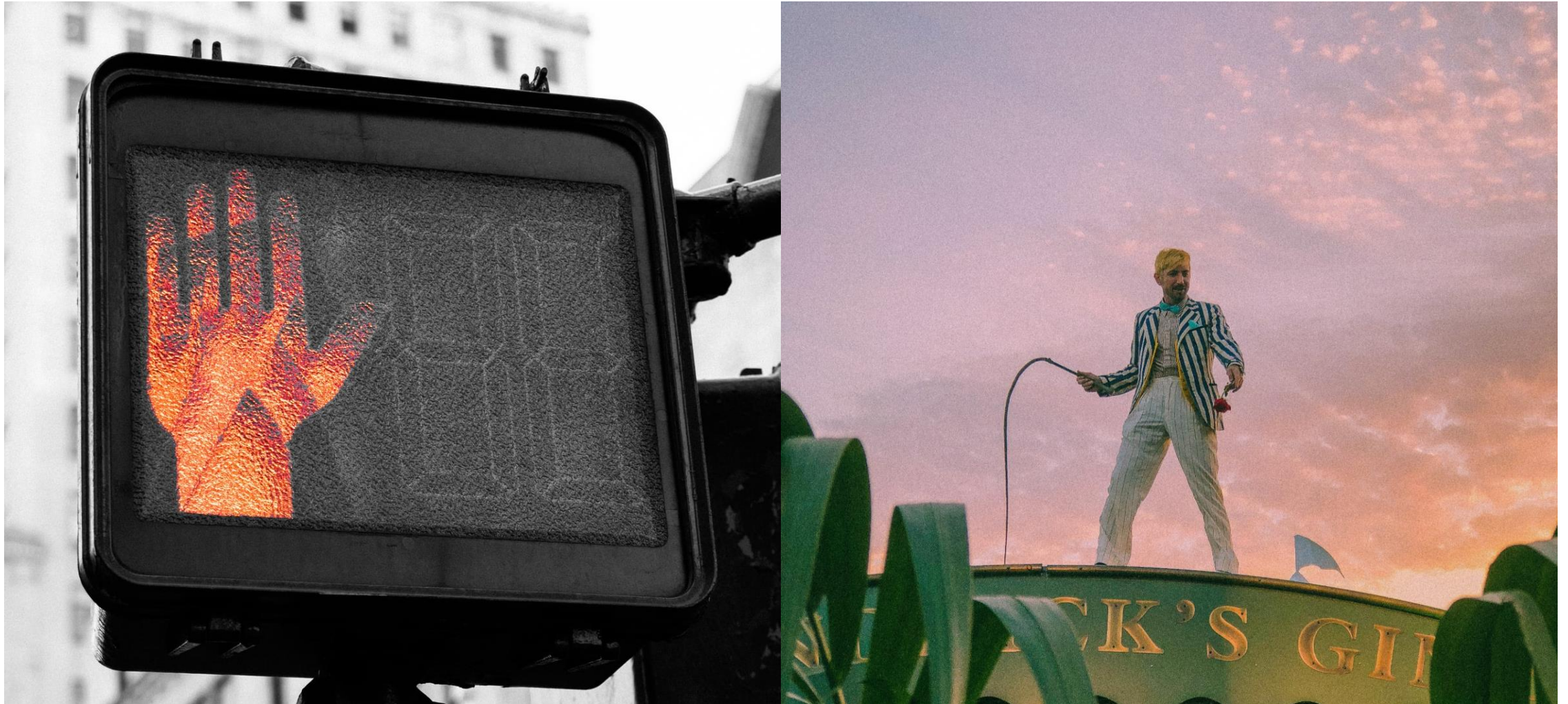
Support for a product might end any time.



Training and instructions are crucial for success.



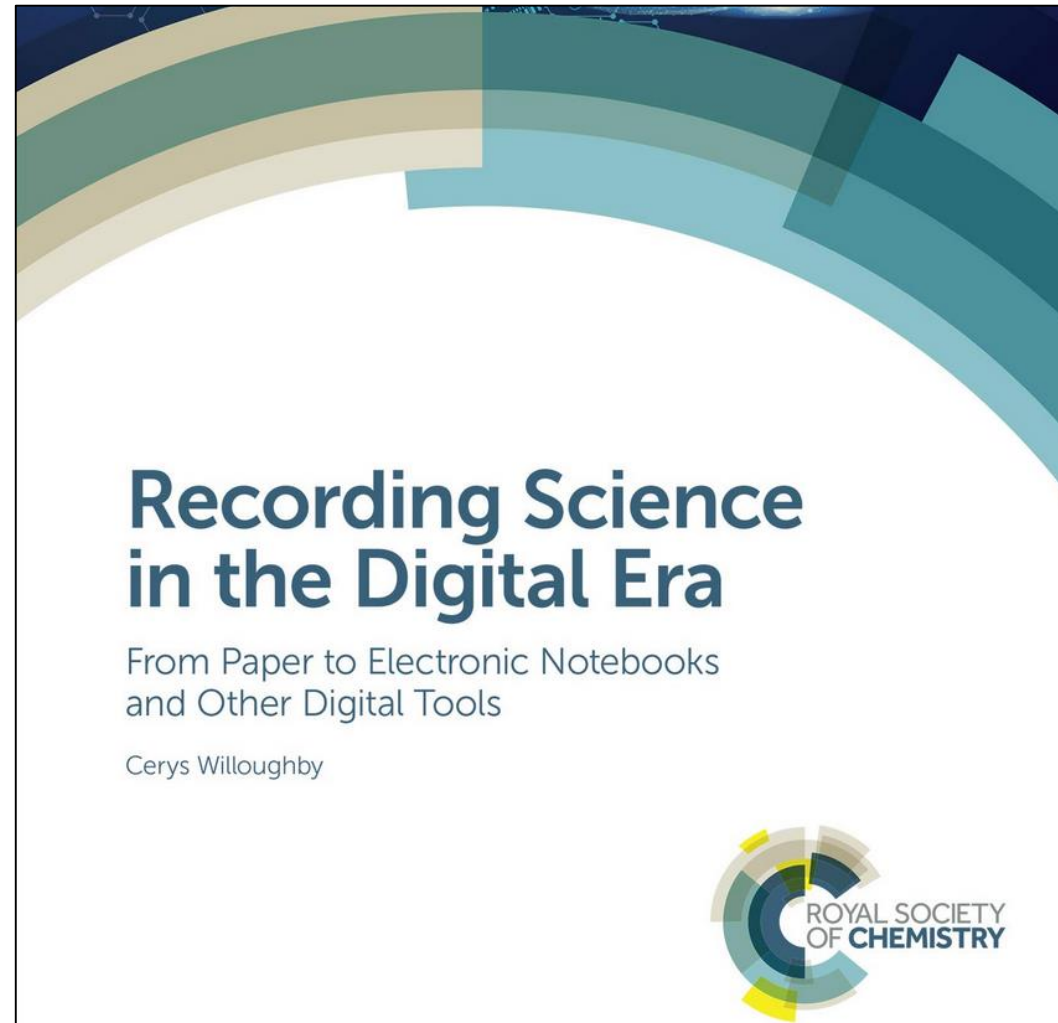
Standards will need to be enforced.



Patience is important



Further Reading



The team of the Chemistry | Biology | Pharmacy Information Center



Dina Idrizovic



Inge Vetsch



Pascal Hauenstein



Dr. Maria Pechlaner

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Regula Furegati



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Dr. Jozica Dolenc



Dr. Leo Betschart



Dr. Oliver Renn

Thank You

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