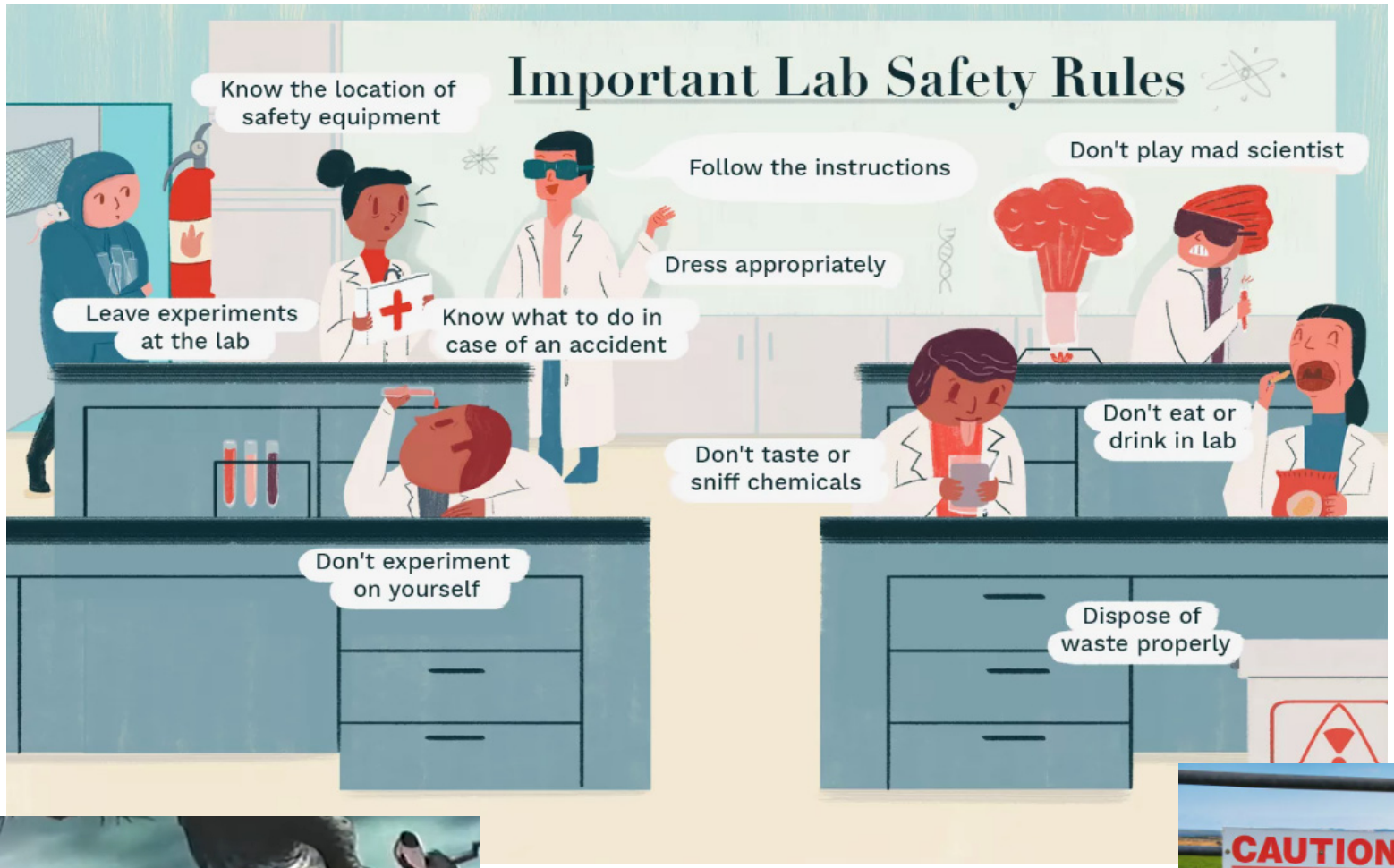
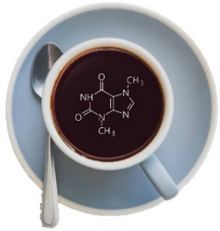


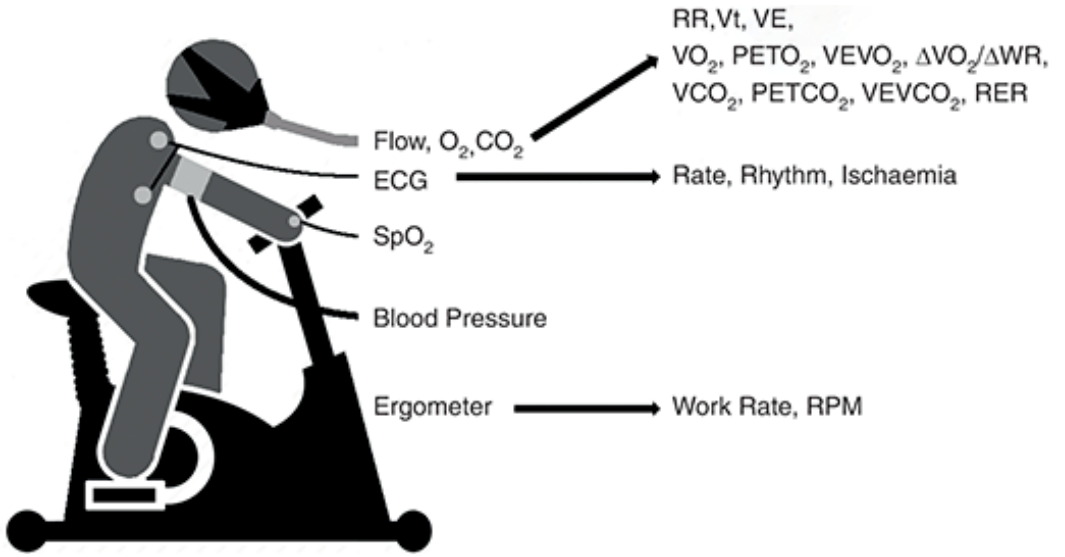
"Are you kiddin'?
There's teeth in the other end."

Caffeine Safety

- To test the impact of caffeine on sport performance
- Two undergraduate student volunteers



https://www.istockphoto.com



https://www.cambridge.org

Caffeine Safety

- New protocol
  - Bulk caffeine versus tablets
- Calculation error; 300 mg -> 30 g
  - Decimal place error (100x)
  - Calculated vaporously; not written or checked
- Medical emergency
  - Dialysis, loss of 22-26 lbs, students recovered
- Court: Lack of supervision – inexperienced / incompetent
- University fined £400,000 ($500,000) + expenses

Caffeine Safety

- If you were the student volunteer, how would you ensure that this would not happen to you?

- If you were the TA/lab coordinator (or classmate, professor/instructor, department head), how would you ensure that this type of error does not happen in the teaching program?

TEXAS TECH UNIVERSITY

'The Accident'

- Preston Brown, fifth year graduate student, training newer student
- Working with ~5 g nickel hydrazine perchlorate (**explosive**) under hexane
- Used mortar & pestle to gently remove clumps
- Removed PPE & was working at bench
- One last stir – mortar **exploded**
- Brown lost three digits on left hand, lacerated right hand & perforated left eye

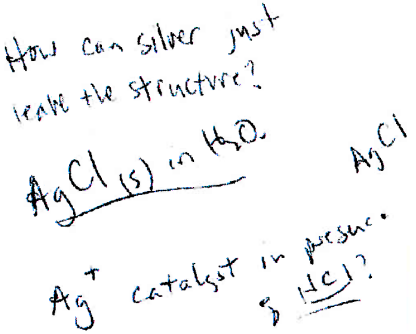
Leading to 'The Accident'

- Labmates were disturbed by [Brown's] conduct in the lab prior to the incident. His space was **disorganized**, items were **not labeled**, and "there had been **conflicts** over work space, **cleanliness** of the lab and use of **chemicals**"
- Brown started scaling up syntheses [eight months before accident], first to 1 to 3 g and then to 5 g
- Colleague told Brown the **scale-up was inappropriate**; Brown reportedly responded that things were "just fine."
- **Colleague** apparently **failed** to report the scale-up to either Weeks (PI) or Hope-Weeks (Co-PI)

Leading to 'The Accident'

- Brown **transported** as much as "several grams of compounds" at a time in glass vials in a backpack or coat pocket
- Weeks (PI) told police that a student reported to him that Brown "would often avoid necessary steps to characterize compounds in order to save time"
- Several vials of material were at Brown's home, **unlabeled**
  - Destroyed by authorities
- Many laboratory vials were **unlabeled**
- **Laboratory notebook** provides no detail

Lab notebook entry



Contributing to The Accident

- Studying energetic or **explosive** compounds
  - 'Improvised' explosives
  - Nickel hydrazine perchlorate
- 'Make no more than 100 mg' – synthesized 10 g
  - **Policy not formalized** or **enforced** in laboratory
- **No records** of syntheses and dispositions
- Wear **PPE**, practice safety – **inconsistent**
- Insufficient safety accountability by PI, Department & University
- No formal **training** for students

Brandon Weeks

Louisa Hope-Weeks

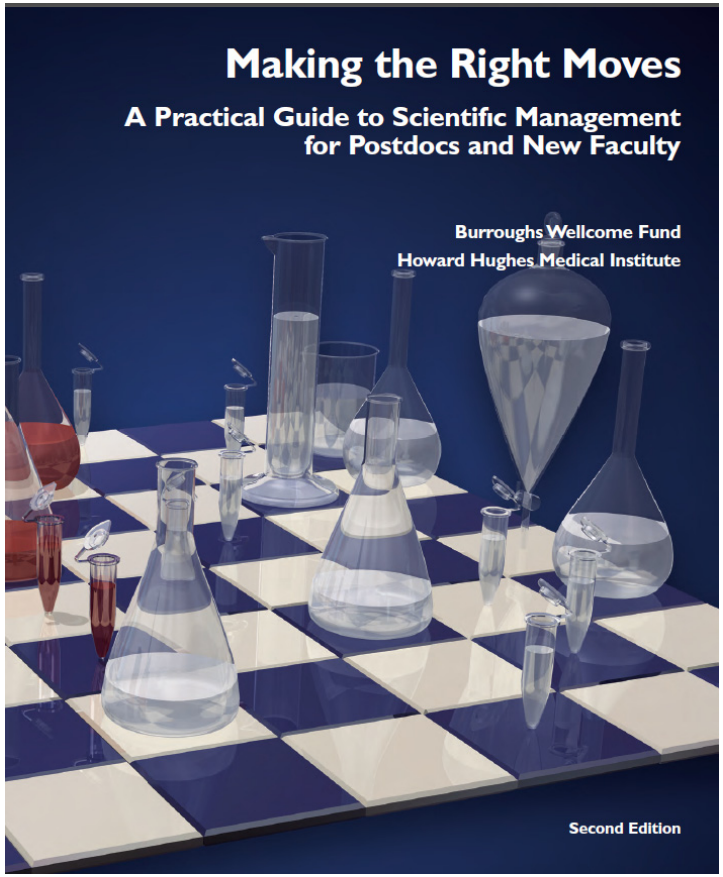
Avoiding an Accident

- What is the role of each of these persons in promoting and ensuring safety in the laboratory?
  - New researcher (i.e., you)
  - Colleagues (other students, including grad students)
  - Laboratory manager
  - Primary investigator
  - Department head
  - Dean (Associate Dean for Research)
  - Vice President for Research
  - Others

Laboratory Safety - Reflection

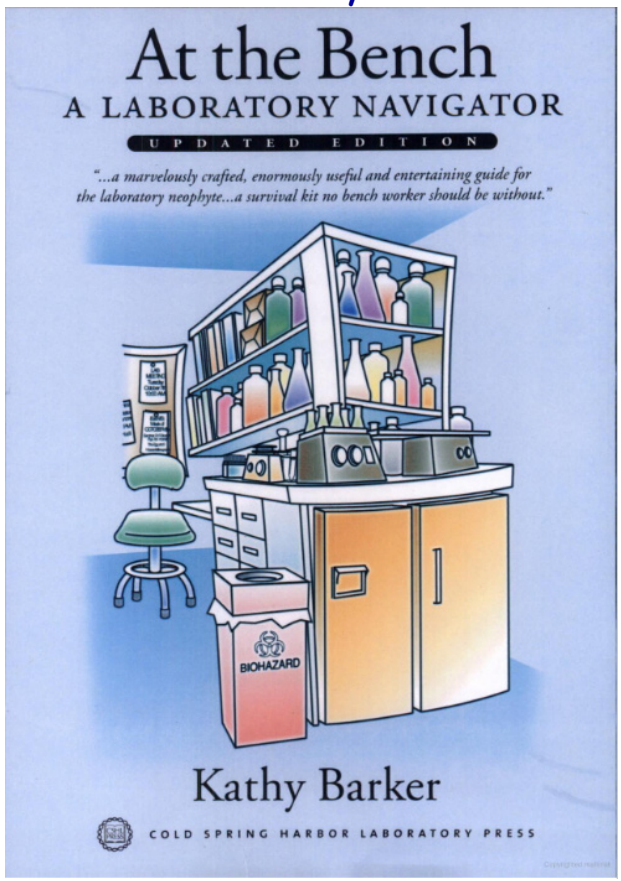
- **Communicate** with mentor and co-workers
- Complete all **safety training**
- **Know your environment** - Risks, engineering controls
- **Wear appropriate PPE** & use safety devices
- **Follow laboratory policies** & SOPs
  - Know and practice protocols
- **Expect** colleagues to be safe
- **Record** aims, goals, preparations, calculations, activities outcomes and conclusions
- **Laboratory notebooks** are legal documents

Records, Data Storage & Security



Chapter 8: Data Management and Laboratory Notebooks

Chapter 5: Laboratory Notebooks



Excellent guides to ~~survive~~ flourish in the laboratory environment

Why Keep a Laboratory Notebook

- Provide a complete record of why experiments were initiated and how they were performed, outcomes, insights & conclusions (**self**)
- Encourage sound thinking. A forum to talk to yourself, to ask questions, to record important thoughts about experimental design & interpretation
- Provide information to persons interested in continuing your research. Others may want to repeat and extend your experimentation **if you die an early death**
  - Complete record of rationale, procedures, reagents, data, and thoughts to bequeath (**others**)
  - Notebooks that are kept solely for personal consumption are often illegible and incoherent (usually both) and are worthless to the broader scientific community
- **To get rich! $$** You may discover or develop something important and in such an event you must have a notebook that supports your claims. If you have not kept up a proper laboratory notebook, other researchers and their patent lawyers will beat you to the Patent Office and to the bank.

modified from https://colinpurrington.com/tips/lab-notebooks/ & Dr Kurt Kwast (University of Illinois)

Why Keep a Laboratory Notebook

Scientific

- Reproducibility
- Publications
- Grant proposals

Legal

- Grants & Contracts
- Quality Assurance
- Product Approval
- Patents
  - Supporting data
  - Dates
  - Proof of practice

modified from Dr Kurt Kwast (University of Illinois)

Essential Elements

Useful Books Explain

- What you did
- Why you did it
- How you did it
- When you did it
- Where materials are
- Outcomes with locations
- Your interpretations
- Contributions

Good Books are

- Legible
- Organized
- Accessible
- Accurate
- Complete
- Secure
- Allow repetition of experiments
- Compliant with granting agencies AND institutional requirements

modified from Dr Kurt Kwast (University of Illinois)

Information to Record

- **Date** (& experiment name or number)
- **Purpose**, hypothesis & goal
- How you did it? (**approach & methods**)
  - Sources of **materials** (vendor, lot #'s, etc.) & preparation
  - **All calculations with units for all components** (e.g., mass, volume, concentration)
  - Self-references to lab-made or proprietary **reagents** (notebook & page)
  - **Organisms**: type, line, passage, generation, age, last fed, etc.
  - **Conditions**: temperature, atmosphere, pH, osmolality, etc.
  - Can refer to centralized methods notebook with version number
    - Must include verification of timing, protocol steps, QA parameters, etc.
  - **Collaborators** – who helped? Reference to their notes

modified from https://colinpurrington.com/tips/lab-notebooks/ & Dr Kurt Kwast (University of Illinois)

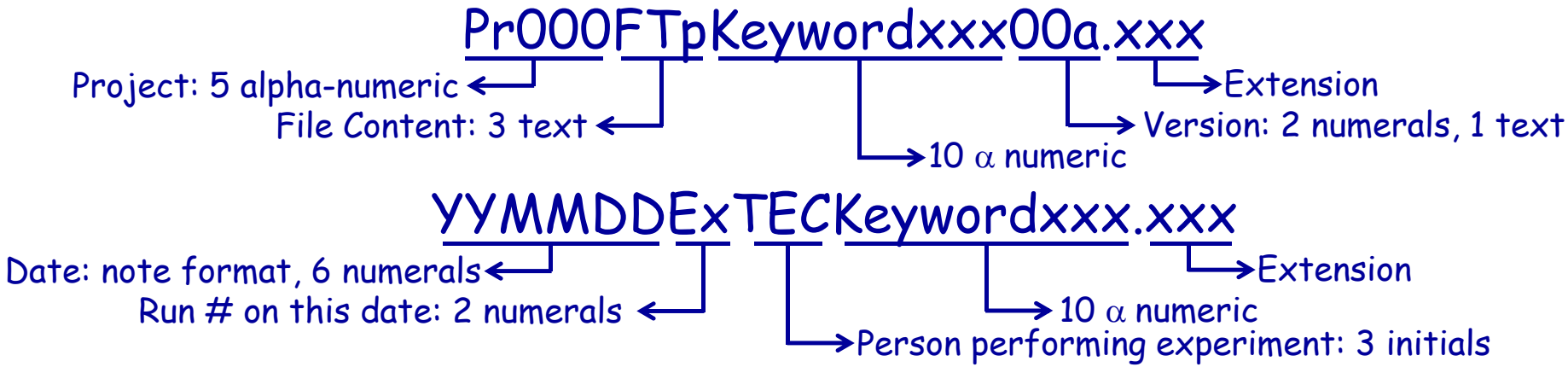
Information to Record

- **Results** (Data/observation/location of generated materials)
  - **Tangible** (photographs, radiographs, printouts, etc. pasted in or location)
  - **Intangible** (qualitative assessment, descriptions, calculations)
  - **Electronic** file names and storage location(s); Derivative files
- May allow space for **comment** when data are reviewed or distilled
- Discussion
  - Can be about any of the above topics (i.e., not just as conclusions)
- **Conclusions**/objective interpretation
  - **Include any artifacts or errors made or observed**
  - Reflect back to hypothesis and goal
- What's next (a.k.a. future directions)?
  - Next experiments / Optimizations / Modifications

modified from https://colinpurrington.com/tips/lab-notebooks/ & Dr Kurt Kwast (University of Illinois)

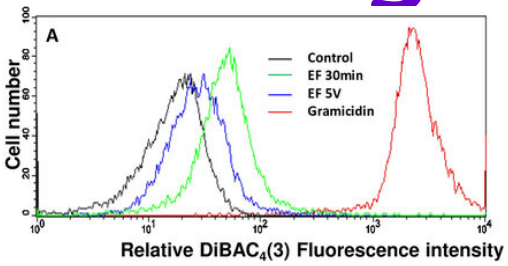
Naming Electronic Files

- File must be accessible & stable
  - Software available to access, manipulate & analyze data
  - Naming must be interpretable by others who will access the information
  - Data archive file unchanged by accessing, copying or compressing
- Name must be unique, meaningful and logical (searchable)

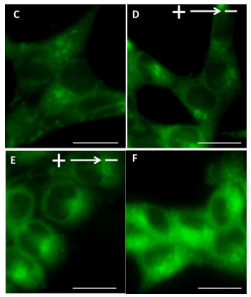


Example: 25052101bdsF508bicarb.csv

Naming & Storing Electronic Files



FACS



Images

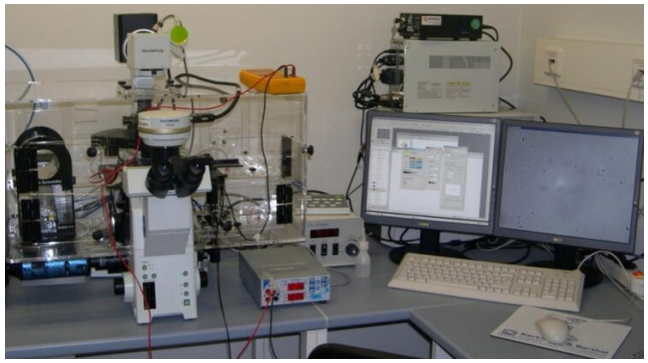
Archive data

16 TB RAID

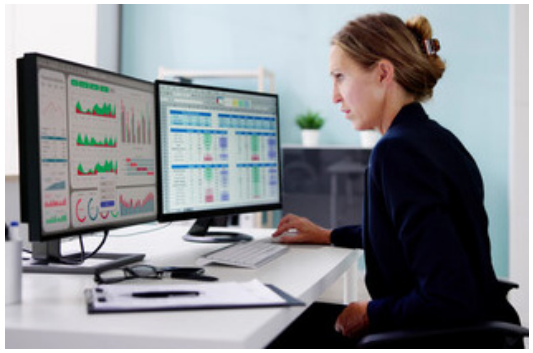
Lab Archives

Organize	Access
Date	New
User	Read
Project	Write
Agency	Modify
Organism	Re-name

Three Trts; Two Time Pts; x.std or x.prp

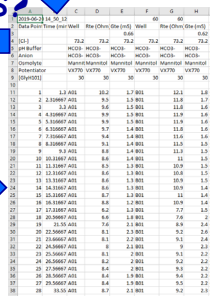


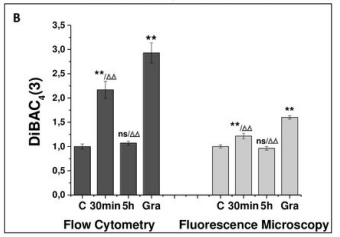
Data Acquisition Systems



Analysis, Distillation, Aggregation, Presentation, Summary , Discussion

Named?
Stored?
Access?





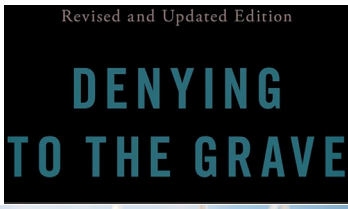
Intermediate & Final Derivative Files
(.prp), .csv, .dat, .txt, .pdf
.jpg, .tif, .psd, .jnb, .doc, .docx .xls

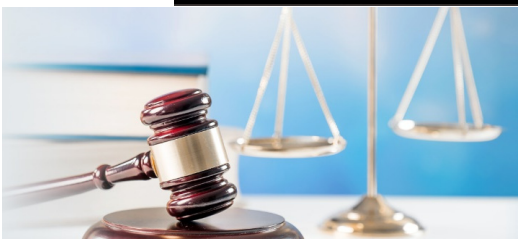
Images: Guerra-Huhne et al. Front Biosci 27: 273, 2022.

Ownership & Access

- Grants:
  - Typically, the grantee 'institution' (e.g., university) owns all data, including laboratory notebooks
  - Primary investigator/Program director responsible for recording, organizing and **securing** data
  - Granting organization may require [open] access to data files and/or submission of information to repositories
  - Granting organization may require access to data, including notebooks, at will (e.g., audit)
- Contracts
  - Typically, contracting agency (e.g., corporation) owns all data, including laboratory notebooks
    - May affect opportunity to use data for future projects or for publication
  - Primary investigator/Program director responsible for recording, organizing, **securing and delivering** data

$$ Record-keeping - Reflection





- Laboratory notebooks are really important!
- What, Why, How, When, Where, Outcomes, Interpretations, Contributions
- Legible, Organized, Accessible, Accurate, Complete, Secure
- Include all calculations!
- Cataloging within a system is really important!
  - Develop effective expandable system to name and organize items
  - Access to reagents and products
  - Access to archival, intermediate and derivative files