



Caffeine Safety



- · To test the impact of caffeine on sport performance
- Two undergraduate student volunteers
- Calculation error; 300 mg -> 30 g
 - Decimal place error (100x)



- new protocol tablets versus powder
- · 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 accident does not happen in the teaching program?







'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





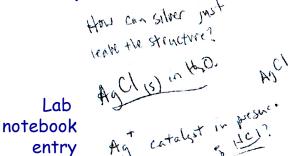
Leading to 'The Accident'

- 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 did not 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





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)
 - -Lab manager
 - -PI
 - 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



Age-Old Conflicts (& Impacts)







Dr Bill, PI



Collaborator













Sci Adv Bd \$12,000+



Image sources availab

K-State COI

Ownership: Ownership interest in any corporation, partnership, trust, joint venture, and every other business interest, including land used for income which you or other members of your household own or have owned within the preceding 12 months, which represents a legal or equitable interest exceeding \$5,000 or five percent, whichever is less. Ownership of intellectual property, e.g., patents, royalties, and copyrights is also included. Ownership of funds and holdings acquired through the Regents' retirement programs is not included.

Are there any ownership interests you have or a member of your family has which meet this criteria? Yes No

Remuneration: Receipt of salary, compensation, fees, commission, anything of value, or economic benefit conferred within the past 12 months in return for services rendered or to be rendered from one or more outside entities, in excess of \$5,000.

Office: A position or office of director, officer, associate, partner, or proprietor in any outside entity in which greater than 5% ownership is held or for which more than \$5,000 compensation is received.

Financial Interests Received From any Foreign Entity: Receipt of salary, anything of value, or economic benefit, including sponsored travel, conferred within the past 12 months, or will occur in the next 12 months, received or to be received from any foreign entity, including governments and universities, in return for services rendered or to be rendered. This includes fees received from private consulting or other international business activities, from any one entity or any government.

Conflict of Time Commitment: As discussed on the introductory page, as an employee you must disclose actual and potential conflicts of time.

Have you engaged in any activity (not previously disclosed) or do you expect to engage in any activity in the future that could impact or appear to impact your primary professional responsibility to K-State, your primary commitment of time and intellectual effort to K-State, and/or your presence on campus commensurate with your appointment? Some examples may include consulting, outside employment, public service, pro bono work, or serving as an officer of an external entity, even without compensation.

K-State Policies and Procedures Manual

Consensual Romantic Relationships Involving Students

Chapter 4094

To protect the integrity of the University academic environment, consensual romantic relationships between employees and students are prohibited when the employee has direct evaluative or supervisory authority over the student. In such instance when a relationship arises contrary to this policy, the employee shall immediately disclose the relationship to the employee's supervisor or department/unit head. The employee shall cooperate with the supervisor, in conjunction with department/unit head as necessary, to sever the evaluative or supervisory relationship and eliminate the existing or potential conflict of interest. A violation of this policy may lead to disciplinary action as appropriate, up to and including termination of employment.

Individuals who believe in good faith that this policy has been violated should report the violation to the employee's supervisor or other appropriate University official.

Nepotism and Employee Relationships

Chapter 4095

If a person is in a position which requires an evaluation or a personnel decision such as those concerning appointment, retention, promotion, discipline, transfer, tenure or salary of a family member, someone with whom such person is in a consensual romantic relationship, or a member of such person's household, such condition shall be deemed a conflict of interest and that person shall not participate in such a decision, and that person shall not participate in any group or body which is considering any such decision.

Age-Old Conflicts & Reflection



- · Communicate
- Transparency
- Trust
- Team

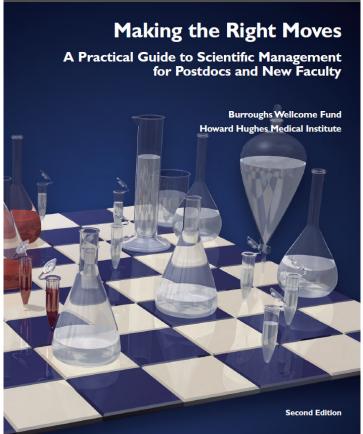


- Percent Effort cover commitments
- Know Goals & Endpoints
- Know & Follow Policies
- Keep complete records



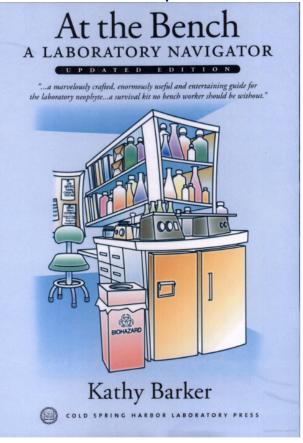


Records, Data Storage & Security



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.

Why Keep a Laboratory Notebook

Scientific

- Reproducibility
- Publications
- Grant proposals

Legal

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

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

How to Record

- Person #1: likes to write with a pencil because it is easy to correct mistakes.
- Person #2: likes to write results on paper towels before transferring to notebook because it is more convenient, and if the experiment does not work, he/she doesn't have to clutter up his/her notebook
- Person #3: keeps a very neat and complete notebook. When he/she makes a mistake, it's carefully obliterated permanently with a magic marker so there is no confusion.

Pen	Abuse treatment						
	Control	Erasure	Water	Methanol	Ethanol	Acetone	Baked
Bic Accountant fine point (red)	123	123	123	-3-1	23	123	123
Bic Accountant fine pt (black)	123	123	123				123
Bic Round Stic med (black)	123	123	123	123	12.3	123	123
Cross fountain pen (blue/black)	123	123	123	123	123	123	123
Dixon Ticonderoga 1388-2 soft pencil	123		123	123	123	123	123
Pentel Hybrid Gel Roller (black)	123	123	123	123	123	123	123
Pilot G-2 07 (black)	123	123	123	123	123	123	123
Sakura Gelly Roll fine (black)	123	123	123	123	123	123	123
Sakura Gelly Roll fine (blue)	123	123	123	123	123	123	123
Sakura Gelly Roll XPGB (blue)	123	123	123	123	123	123	123
Sakura Gelly Roll XPGB (green)	123	123	123	123	123	123	123
Sakura Gelly Roll XPGB (red)	123	123	123	123	123	123	123
Sakura Pigma Micron .45 mm (black)	123	123	123	123	123	123	123
Sanford Sharpie extra fine (black)	123	123	123	125	123	523	123
Sanford Sharpie extra fine point (red)	123	123	123	146		127	123
Sanford Sharpie ultra fine point (blue)	123	123	123				123
Sanford Uni-Ball Gel RT Med (black)	123	123	123	123	123	123	123
Sanford Uni-Ball Vision fine (black)	123	123	123	123	123	123	123
Sanford Uni-Ball Vision fine (blue)	123	123	123	123	123	123	123
Sanford Uni-Gel RT fine (blue)	123	123	123	123	123	123	123
Zebra Sarasa 0.7 (blue/black)	123	123	123	123	123	123	123

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

Information to Record

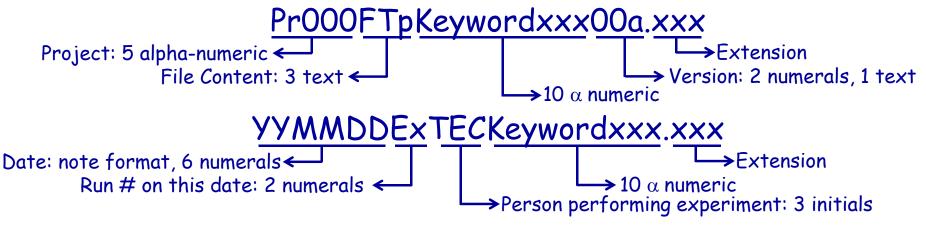
- Date (& experiment name or number)
- Purpose, hypothesis & goal
- How you did it? (approach & methods)
 - Sources of materials (vendor, lot #'s, etc.) & preparation
 - All calculations with units for all components (e.g., mass, volume, concentration)
 - Self-references to lab-made or proprietary reagents (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

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

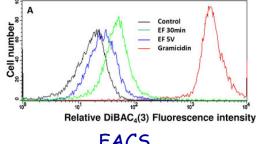
Naming Electronic Files

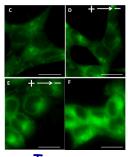
- File must be accessible & stable
 - Software available to access, manipulate & analyze data
 - Naming must be interpretable by others who will access the information
 - Data archive file unchanged by accessing, copying or compressing
- Name must be unique, meaningful and logical (searchable)



Example: 24052101bdsF508bicarb.csv

Naming & Storing Electronic Files





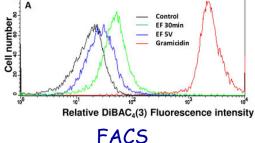
Archive data



Lab Archives

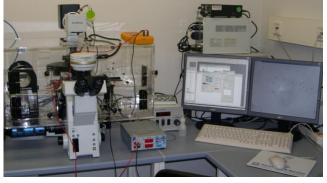
Organize Date User Project Agency Organism

Access New Read Write Modify Re-name





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

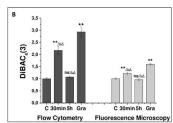


Data Acquisition Systems



Analysis, Distillation, Aggregation, Presentation, Summary, Discussion





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



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, 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

The "Baltimore" or "Imanishi-Kari Case"

David Baltimore - Nobel Laureate (Physiology) at 37!!; tumor viruses and host cell genetics - "co-discovered" reverse transcriptase

Thereza Imanishi-Kari - Assistant Professor, MIT

Margot O'Toole - Postdoc in Imanishi-Kari's lab

Eisen Committee - MIT

NIH Committee

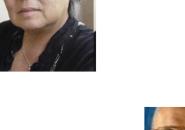
Office of Research Integrity - NIH

John D. Dingell - House Subcommittee on Oversight and Investigation

Secret Service-Dingell sent loose data pages for forensic analysis

Walter Stewart and Ned Fedor - self-appointed "guardians" of scientific integrity; NIH researchers brought to subcommittee staff by Dingell







The "Baltimore" or "Imanishi-Kari Case"

- O'Toole not able to reproduce experiments in 1986 Cell paper ("Altered repertoire of endogenous immunoglobin gene expression in transgenic mice containing a rearranged mu Heavy Chain gene" Cell 1986:45:247-59)
- First Review MIT and Tufts: errors in the paper but no wrong doing;
 alternate interpretations
- Second Review NIH: serious errors but not fraud
- >USSS: concludes 1/3 [of section of notebook entries] altered or out of chronological order
- · ORI finds Imanishi-Kari guilty of 19 counts of research misconduct
 - ten-year embargo; paper retracted; Baltimore steps down as president at Rockefeller
- · Fourth review ORI Appeals Board clears Imanishi-Kari on all counts

Re-identifying Data: Riding with Stars

Ride

Photo

\$10.50 no tip

- 2013 yellow cab data set obtained with FOIA request
 - pickup and drop off times, locations, fare and tip amounts, (hashed) versions of the taxi's license and medallion numbers
- Paired with paparazzi photos to determine trips taken & tips given by selected 'stars' Brad Cooper
- Destinations of trips originating near Larry Flynt's Hustler Club, midnight to 0600
 - ... address revealed resident's name. ... other drop-offs at this address, ... also frequented ... "Rick's Cabaret" and "Flashdancers". Using websites like Spokeo and Facebook, able to find out his property value, ethnicity, relationship status, court records and even a profile picture



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



