Best Practices for Data Management When Using Instrumentation

A tutorial on effective data collection, saving, and processing methods

Created by the Office of Research Compliance and Training
As part of the Research and Data Integrity (ReaDI) Program
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Why Management of Data is Crucial

• Good data management practices keep you organized
  – Data files are easier to locate
  – Less time spent repeating experiments because a data file is unable to be located
  – Reduced time searching for data files when writing publications or thesis

• Some federally funded grants and many publications require data be made publically accessible
  – Well managed data with easily identifiable file names aid in the distribution of data

• Maintaining accurate records provides integrity to research results, defends against accusations of fraud, and supplies proof of intellectual property
Outline

I. Best practices for Labeling the Laboratory Notebook and Naming Data Files
II. Planning Ahead
III. Organization and Collection of Data
IV. Additional Considerations Using Instrumentation and Processing Data
V. Summary
I. Best Practices for Labeling the Laboratory Notebook and Naming Data Files

• This section will introduce:
  – The importance of using a laboratory notebook
  – Notebook labeling practices
  – Data file naming practices
Importance of the Laboratory Notebook

• A laboratory notebook is an important tool because:
  – It is a written record of procedures, reagents, data, calculations, thoughts, explanations, and results of experiments
  – It is a legal document used to defend intellectual property and accusations of fraud
  – It is knowledge for future researchers
  – It is the foundation of a thesis and other publications
Laboratory Notebook: A Researcher’s Tool for Data Organization

• Before getting started with data collection it is important to choose a labeling system for your notebook, and document it.
• A notebook labeling system will be a tool used to reference data collected to a particular entry by the researcher or anybody wanting to view researcher’s results.
• For more information about good laboratory notebook practices refer to the *Good Laboratory Notebook Practices Tutorial*.
Labeling Your Laboratory Notebook

• Check with your PI or lab manager for established conventions for your research group

• On the cover of your lab notebook include, as appropriate:
  – Your name
  – Your position
  – Your PI’s name
  – The title of the project or study
  – Dates the notebook used
  – Volume number

• Label the spine if using a bound notebook
Labeling Your Laboratory Notebook

• Include the same information on the first page of the notebook, along with:
  - Your email
  - Your phone number
  - Your lab and/or office address
  - The abbreviated name by which this notebook will be indicated in file names or other references

This notebook belongs to: Sci N. Tist
Contact information: ST00@columbia.edu
Office #: 212-555-555
Smith Hall
1000 First St. Room 300
NY, NY 01001
Dates used:
Feb 2010-Jan 2011
Notebook #:
IV
Notebook abbreviation:
SNT_IV
Best Practices for Data File Naming

• Check if there are standards that are required by your research group and/or discipline

• Files names should include:
  – Date of data collection (or data file created), listing year first sorts files chronologically
  – Notebook and page number that it refers to
  – If multiple files are being created on the same date and referring to the same sample, notebook, and page number use a numbering (or lettering) code to distinguish between data files
  – Additionally, file names may include the project identification or a brief description

**Identifier:**

<table>
<thead>
<tr>
<th>Date</th>
<th>Notebook/Page #</th>
<th>Sample/Special Notes</th>
<th>Series</th>
</tr>
</thead>
<tbody>
<tr>
<td>20101217</td>
<td>SNT IV 285</td>
<td>Fe2O3_InLens_a</td>
<td></td>
</tr>
<tr>
<td>20101217</td>
<td>SNT IV 285</td>
<td>Fe2O3_InLens_b</td>
<td></td>
</tr>
<tr>
<td>20101217</td>
<td>SNT IV 285</td>
<td>Fe2O3_InLens_c</td>
<td></td>
</tr>
<tr>
<td>20101217</td>
<td>SNT IV 285</td>
<td>Fe2O3_SE2Det_d</td>
<td></td>
</tr>
</tbody>
</table>

**Interpretation:**

**Date Taken:** Dec 17th 2010
**Sci N. Tist:** Notebook IV
**Sample & detector used:** Page 285
**Different files of same sample indicated by continuation of lettering**
Best Practices for Data File Naming, Continued

• Write down the name of the data file in the corresponding notebook to maintain a record of the data file being created

• Consider creating a text file, to be saved in the same folder, that defines the file naming convention

• Some conventions suggest an instrument identification

• Be consistent and document the naming convention that is chosen

• Special consideration needs to be given when naming files with PII (Personally Identifiable Information) or PHI (Personal Health Information). Refer to RASCAL trainings TC0019 or TC0087 for regulations outlined by HIPAA and human subjects research

All of the following would be considered equivalent file names:

20101217_SNT_IV_285_Fe2O3_inLens_a.tif
101217_SNT_IV285_Fe2O3_inLens_a.tif
101217_SNT4_285_Fe2O3inLens_a.tif
Tips for Naming Data Files

• Letters from A to Z and numbers 0 to 9
• Use underscores rather than spaces
• Use brief names (<30 characters)
• Avoid using special characters
  – Ex: \` ‘ = / < > ^ : ; | # * ( ) . ? % , “ @ ! + { } ~ - [ ]
• The 3-letter file extension should be reserved for application-specific codes, e.g., .wrl, .mov, .tif
• Differentiate file name parts using mixed cases or underscores
• When creating a sequentially numbered series of files, use leading zeroes so that they sort properly e.g., file001.txt, file002.txt, file003.txt ... file042.txt
I. Summary

• Check with your PI or lab manager if there are standards for notebook and data file naming. Adhere to the expectations of your PI and research discipline

• Laboratory notebooks should be labeled so that it identifies the researcher and dates used, and if applicable, the research project

• Document your laboratory notebook labeling convention and be consistent

• File names of collected data should include the date of collection, notebook and page number identifier, and a short description

• Once a data file naming format is chosen, write it down and be consistent
II. Planning Ahead

• This section will address
  – Important details to consider before experimentation
  – Notebook preparation
  – Tips for creating data tables
  – Information that needs to be included in the laboratory notebook
Important Details to Consider Before Experimentation

• Before beginning data collection, it is essential to know how the instrument saves and exports data

• Unsure how the instrument saves and exports data?
  – Ask a fellow group member (graduate student, post-doc, staff scientist, etc.)
  – Ask the person who maintains the instrument
  – Practice with an unimportant sample (blank)
Questions Related to Instrumentation

• What file format should data be exported as?
  – Know which file formats are compatible with other operating systems, analyses programs, and data archiving
  – Avoid using file extensions that are unique to a particular software used for data collection. If data are available only in closed or proprietary formats, are there programs available for file migration to a more useful format?
    – Most compatible formats include:
      • ASCII, PDF, .csv, FLAC, TIFF, JPEG2000, MPEG-4, XML, RDF, .txt, .r

• What descriptors should be added? What information will you need to find, identify, or understand the file in the future?
  – Units and other relevant information
  – Independent & dependent variable column headers
  – The ability to add notes or descriptors
Notebook Preparation

Prior to running samples or starting the experiment, make sure you know the answers to the following, and that the answers can be found in the experiment documentation

– How many samples will be looked at?
– How is each sample different?
– What descriptors will you use to distinguish each sample?
– If the same sample is being probed multiple times, what are the varying parameters?
– What is the minimum amount of information that must be recorded to reproduce the experiment?

• Create a table in your notebook with descriptive headers
  – Create a template (can use Word or Excel) that can be re-used each time that particular instrumentation is being used
General Tips for Creating A Table

• Use descriptive labels, including units, in header row, for each column
• The column furthest to the left should be the independent variable (the item that is changing, i.e. your sample)
• Dependent variables should follow in the next columns
• Any derived variables (from calculations) follow the dependent variables. Calculations and formulas need to be documented
• Derived data should reflect the same number of significant figures as the measured values
• If creating a template, the use of formatting (ex: color, boldface, or italicized fonts) can help visually organize data

<table>
<thead>
<tr>
<th>Sample</th>
<th>pH (Trial 1)</th>
<th>pH (Trial 2)</th>
<th>pH (Trial 3)</th>
<th>Average pH</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unfunctionalized WO₃ nanoparticles in H₂O</td>
<td>3.58</td>
<td>3.62</td>
<td>3.64</td>
<td>3.61</td>
</tr>
<tr>
<td>Citric acid modified-TiO₂ nanoparticles in H₂O</td>
<td>5.38</td>
<td>5.44</td>
<td>5.45</td>
<td>5.42</td>
</tr>
</tbody>
</table>

Relevant Information to be Included in Notebook

• Any parameters that are *REQUIRED* to reproduce the experiment need to be recorded
  – E.g.: Substrates, energy output/input, solutions used, background samples, etc.

• Any observations regarding the instrumentation process that would be considered “unusual”
  – E.g.: noise background due to construction, elevated temperatures due to broken AC, etc.

• Any software that is unique to that instrument or a code that has been written for particular types of experiments
  – E.g.: LabVIEW program specifically designed for experiment

• Initial observations while data is being collected

• During data collection, any pre-planned tables should be filled in after each file is created
Example Notebook Entry

2010 December 17

Scanning Electron Microscopy (SEM) images of Fe₂O₃ nanoparticles.

Synthesized 2010 December 15 as referred to on page 282 of this notebook

Instrument Parameters:
Accelerating voltage: 2.0 kV
Used both In-Lens and SE2 detectors
Substrate used: Si-wafer <0.001 Ω

Special notes: construction on floor created some minor difficulty with focusing images

<table>
<thead>
<tr>
<th>Image File Name</th>
<th>Detector Used</th>
<th>Scale Bar</th>
</tr>
</thead>
<tbody>
<tr>
<td>20101217_SNT_IV_285_Fe2O3_InLens_a</td>
<td>In Lens</td>
<td>1 um</td>
</tr>
<tr>
<td>20101217_SNT_IV_285_Fe2O3_InLens_b</td>
<td>In Lens</td>
<td>200 nm</td>
</tr>
<tr>
<td>20101217_SNT_IV_285_Fe2O3_InLens_c</td>
<td>In Lens</td>
<td>2 um</td>
</tr>
<tr>
<td>20101217_SNT_IV_285_Fe2O3_SE2_d</td>
<td>SE2</td>
<td>200 nm</td>
</tr>
</tbody>
</table>

- Thorough description of sample
- Instrument parameters used
- Special notes
- Table that organizes data collected
- Descriptive file name with reference to notebook location
- Where saved data files are located

Data file location in Research Group Archive:
SciNTist_Research → Instrumentation → SEM → 20101217_SNT_IV_285
II. Summary

• Be prepared prior to data collection
• Create a table in notebook to aid in organization of the experiment and data collection
• The notebook needs to contain all the necessary information so that the experiment could be repeated by yourself or other researchers
• Include the data file name in the notebook entry along with the file location
III. Organization of Collected Data

• This section will evaluate the importance of:
  – Archiving data
  – An electronic filing system
  – Use of folders and sub-folders
  – Use of shared computers and portable storage devices
  – Transferring data from a portable storage device to data archive
Archiving Data

• It is essential that a method for archiving data is established prior to any data collection

• It is the responsibility of the PI to maintain archived data; check with your PI on the procedures for storing and saving data

• Archived data should be secured as required by University policies and procedures, and state, and/or federal regulations

• Archived data should be in one location that is accessible by all group members and/or collaborators (e.g.: research group drive, online repository, etc.) with at least two back-ups
  – In addition to the file on the local machine, there should be one copy backed up on a separate local system, and one copy held at a geographically distant location

• For more information regarding data management and storage, please visit (Insert RDM tutorial link by Joel and Amy)
Electronic Filing System for Data Organization

• Before data collection, it is important to determine an electronic filing system that best suits your research project
• The use of a filing system helps organize collected data
• Within the archive, it may be useful to create an “Instruments” folder; at a minimum, a file for EACH type of instrument used to collect data should be created
• If more than one of the same type of instrument is used, but in a different facility, with different capabilities, etc., use underscores to help identify each one
  – It is extremely important to document where each data set originates, for reproducibility of experiments
Organizing Sub-folders

- Within each instrument folder, create a new folder in which all the data collected can be organized
- Use of sub-folders helps keep data organized for easier referral
- Name sub-folders using date, descriptions, notebook identifiers, etc.
  - Remain consistent with the names of sub-folders

Within the NMR_Hermes folder, sub-folders have been created

Folders are labeled with date, notebook reference, and brief sample description

Each folder contains data related to this particular sample, e.g.: $^1$H-NMR, $^{13}$C-NMR, COSY, etc.
Collecting Data Using Portable Data Storage

- Many instruments are connected to a computer that is shared with many other researchers from different groups and disciplines
- If privileges are allowed, create a folder on the shared computer with your name to use as temporary storage while collecting data
- **Do not** use shared computers for permanent (long-term) data storage
- Whenever possible, save data to a secure server that employs regular backup protocols, with quality control check
- A portable flash drive can be used to remove data from shared computers to a permanent storage location
- Use same folder and sub-folder organization on portable flash drive
- Use password protected flash drive if saving sensitive data
Transferring Data to a Permanent Location

- Flash drives should never be used as permanent storage.
- Using the same folder and sub-folder organization facilitates transfer of data:
  - Click and drag (or copy and paste) data files into correct folders on data archive.
- Never delete data from portable device until data has been transferred and can be confirmed by either opening data file and/or using a checksum algorithm.

![Diagram of data transfer process with copy and paste highlighted.](image)
III. Summary

• A data archive system with multiple data back-ups should be established by the PI of the research group
• Creation of folders for different types of instrumentation keeps data files organized
• Use of sub-folders allows for easier referral to collected data files
• Portable flash drives are not meant for permanent data storage
• Data collected on portable devices should be transferred to a data archive ASAP
• Special requirements govern the proper handling of human subjects data
IV. Additional Considerations
Using Instrumentation and Processing Data

• This section will provide recommendations for the following scenarios:
  – Use of instrumentation with user modified software and/or programming
  – Use of instruments that have limited ability describing data being collected
  – Processing multiple data sets
  – Instrumentation ethics
Instruments That Allow Additional Remarks

- Some instruments have multiple ways of allowing additional comments within the program
- If you choose to utilize these options, then:
  - Be aware that these comments are often not exportable to another file format, and that the original proprietary program may be required to view these comments
  - Be sure to record ALL comments about the data file in your notebook as well
  - Do not use this option to replace descriptive comments in your notebook
  - Do not use this option to replace descriptive data file names

<table>
<thead>
<tr>
<th>Commands</th>
<th>Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cyclic voltammetry potentiostatic</td>
<td>Cyclic voltammetry potentiostatic</td>
</tr>
<tr>
<td>Remarks</td>
<td>Options</td>
</tr>
<tr>
<td>End status Autolab</td>
<td>Time, WE(1).Potential, WE(1).Current</td>
</tr>
<tr>
<td>Signal sampler</td>
<td>1 Options</td>
</tr>
<tr>
<td>Options</td>
<td></td>
</tr>
<tr>
<td>Instrument</td>
<td>Instrument description</td>
</tr>
<tr>
<td>Instrument description</td>
<td></td>
</tr>
<tr>
<td>Autolab control</td>
<td></td>
</tr>
<tr>
<td>Set potential</td>
<td>0.000</td>
</tr>
<tr>
<td>Set cell</td>
<td>On</td>
</tr>
<tr>
<td>Wait time (s)</td>
<td>5</td>
</tr>
<tr>
<td>Optimize current range</td>
<td>5</td>
</tr>
<tr>
<td>CV staircase</td>
<td>[0.000, 1.000, -1.000, 0.000, 2, 0.1000000]</td>
</tr>
<tr>
<td>Set cell</td>
<td>Off</td>
</tr>
</tbody>
</table>

- The user is able to include any identifiers about the sample
- The “Data View” option in this program allows the remarks to be seen; useful for quick analysis
- The remarks are not exported with the data file
Unique Software and Programming

When using software like LabVIEW to write a specific program, it is important to:

– Record in notebook the EXACT methods and codes used, including hand-drawings and/or printed-out images affixed to laboratory notebook page

– Describe the different elements used, including model numbers if applicable

– Save the file so that it can be referred to the notebook entry

This LabVIEW was created on Feb. 7, 2009 to measure torque parameters and can be referred to page 45 in Sci N. Tist’s notebook #3

http://www.nyu.edu/classes/mcdonough/m&ei.htm
Instruments That Assign Default File Names

- Some instruments do not allow users to give file names, but generate a default name.
- For these types of instruments, it is useful to include an additional column in your table to record the default name given, then rename files later.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Excitation wavelength</th>
<th>Pulse Energy (mJ)</th>
<th>Saved As</th>
<th>Renamed As</th>
</tr>
</thead>
<tbody>
<tr>
<td>10 nm Ni Nanoparticles SNT_V_32</td>
<td>400 nm</td>
<td>0.100</td>
<td>Print_01</td>
<td></td>
</tr>
<tr>
<td>20 nm Ni Nanoparticles SNT_V_15</td>
<td>550 nm</td>
<td>0.050</td>
<td>Print_02</td>
<td></td>
</tr>
<tr>
<td>75 nm Ni Nanoparticles SNT_V_40</td>
<td>600 nm</td>
<td>0.100</td>
<td>Print_03</td>
<td></td>
</tr>
</tbody>
</table>
Renaming Default File Names

- Default names give no description of the data they contain
- Rename data files ASAP using notebook table as guidance
  - Right-click file and select rename option or file renaming tools for multiple files
- Use a file name that is descriptive, so the files are easier to find for later referral

<table>
<thead>
<tr>
<th>Sample</th>
<th>Excitation wavelength</th>
<th>Pulse Energy (mJ)</th>
<th>Saved As</th>
<th>Renamed As</th>
</tr>
</thead>
<tbody>
<tr>
<td>10 nm Ni Nanoparticles SNT_V_32</td>
<td>400 nm</td>
<td>0.100</td>
<td>Print_01</td>
<td>20110914_SNT_V_32_10nmNiNPs_400nm_Excite</td>
</tr>
</tbody>
</table>

Use of additional column for renamed filename
- maintains organization
- maintains a written record in notebook of data file being created
- simplifies reference when searching for electronic data files
### Processing Data

- Some data sets require further manipulations after collection (e.g., baseline correction, background subtraction, etc.). These transformations cannot take the place of raw data.
- Never alter the raw data set
  - Indicate that it is the raw data in the file name
  - Save each data manipulation with its own unique file name
- If working with multiple data sets in one spreadsheet or database, use descriptive titles that refer to the raw data file.

#### File name of data and brief description

Explains how data was manipulated

Describes the instrument parameters, date, and dependent variables

<table>
<thead>
<tr>
<th>Independent variable and instrument background</th>
<th>Voltage (mV)</th>
<th>File name of data and brief description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time (sec) Dark Background Noise Signal</td>
<td>20100401_SNT_IV_34 100 nm SnO₂ Nanorods Synthesized 20100329</td>
<td>Measured Photovoltage at 350 nm excitation for different SnO₂ samples, taken 20100401</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Time (sec)</th>
<th>Voltage (mV)</th>
<th>File name of data and brief description</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00E+00</td>
<td>1.0547E-04</td>
<td>20100401_SNT_IV_34 100 nm SnO₂ Nanorods Synthesized 20100329</td>
</tr>
<tr>
<td>5.00E-10</td>
<td>1.4453E-04</td>
<td>20100401_SNT_IV_34 100 nm SnO₂ Nanoparticles Synthesized 20100315</td>
</tr>
<tr>
<td>1.00E-09</td>
<td>1.2199E-04</td>
<td>20100401_SNT_IV_34 100 nm SnO₂ Nanorods Background Subt (C#-B#)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Time (sec)</th>
<th>Voltage (mV)</th>
<th>File name of data and brief description</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00E+00</td>
<td>2.8320E-03</td>
<td>20100401_SNT_IV_34 100 nm SnO₂ Nanorods Synthesized 20100329</td>
</tr>
<tr>
<td>5.00E-10</td>
<td>2.9297E-03</td>
<td>20100401_SNT_IV_34 100 nm SnO₂ Nanoparticles Synthesized 20100315</td>
</tr>
<tr>
<td>1.00E-09</td>
<td>3.1250E-03</td>
<td>20100401_SNT_IV_34 100 nm SnO₂ Nanorods Background Subt (C#-B#)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Time (sec)</th>
<th>Voltage (mV)</th>
<th>File name of data and brief description</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00E+00</td>
<td>1.2793E-03</td>
<td>20100401_SNT_IV_34 100 nm SnO₂ Nanorods Synthesized 20100329</td>
</tr>
<tr>
<td>5.00E-10</td>
<td>1.4258E-03</td>
<td>20100401_SNT_IV_34 100 nm SnO₂ Nanoparticles Synthesized 20100315</td>
</tr>
<tr>
<td>1.00E-09</td>
<td>1.9531E-03</td>
<td>20100401_SNT_IV_34 100 nm SnO₂ Nanorods Background Subt (C#-B#)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Time (sec)</th>
<th>Voltage (mV)</th>
<th>File name of data and brief description</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00E+00</td>
<td>2.7266E-03</td>
<td>20100401_SNT_IV_34 100 nm SnO₂ Nanorods Synthesized 20100329</td>
</tr>
<tr>
<td>5.00E-10</td>
<td>2.7852E-03</td>
<td>20100401_SNT_IV_34 100 nm SnO₂ Nanoparticles Synthesized 20100315</td>
</tr>
<tr>
<td>1.00E-09</td>
<td>3.0039E-03</td>
<td>20100401_SNT_IV_34 100 nm SnO₂ Nanorods Background Subt (C#-B#)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Time (sec)</th>
<th>Voltage (mV)</th>
<th>File name of data and brief description</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00E+00</td>
<td>1.1738E-03</td>
<td>20100401_SNT_IV_34 100 nm SnO₂ Nanorods Synthesized 20100329</td>
</tr>
<tr>
<td>5.00E-10</td>
<td>1.2812E-03</td>
<td>20100401_SNT_IV_34 100 nm SnO₂ Nanoparticles Synthesized 20100315</td>
</tr>
<tr>
<td>1.00E-09</td>
<td>1.8320E-03</td>
<td>20100401_SNT_IV_34 100 nm SnO₂ Nanorods Background Subt (C#-B#)</td>
</tr>
</tbody>
</table>
Instrumentation Best Practices

• A written record (either paper or digital) should be used to record who used the instrument and when. Be sure to fill out the log accurately

• In the logbook, record any malfunctions, maintenance performed, changed settings, etc.

• Most instruments are equipped with security controls, which identifies person and timestamp. These should NEVER be disabled

• Each user/group should have unique login and password. NEVER share your password, especially with unauthorized users

• Login and logbook information provides “audit trail” of instrument usage
Summary of Best Practices for Data Management Using Instrumentation

1. Always check with your PI about expected standards to be followed by all group members
2. Use documented notebook and data file naming conventions to keep data organized
3. Prepare notebook prior to the beginning of experimentation
4. Use a table to organize data as it is collected
5. Organize data using electronic filing system with descriptive folder and sub-folder names
6. Use portable storage only as TEMPORARY means to transfer data to a permanent location
7. Understand the capabilities of instruments regarding exporting data files
8. When processing data, never alter raw data sets
9. Use clear descriptors if combining multiple data sets to one spreadsheet
10. Use instrument logbooks and do not share login information
Additional Resources and Further Reading:

- Tutorial on *Good Laboratory Notebook Practices*
- Tutorial on *Data Management*
- RASCAL trainings TC0019 and/or TC0087 for PHI, PII
- Laboratory notebook and data file naming best practices:
  - [http://datalib.edina.ac.uk/mantra/libtraining/Session2GroupExercise1.pdf](http://datalib.edina.ac.uk/mantra/libtraining/Session2GroupExercise1.pdf)
  - [http://uresearch.miami.edu/?p=103&s=25](http://uresearch.miami.edu/?p=103&s=25)
  - [https://www.training.nih.gov/assets/Lab_Notebook_508%28new%29.pdf](https://www.training.nih.gov/assets/Lab_Notebook_508%28new%29.pdf)

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