

**Project Title:**

Training modules for improving the reproducibility of experimental data recording and pre-processing with examples from microbiology and immunology

## Cover Letter:

Please accept the attached grant “Training modules for improving the reproducibility of experimental data recording and pre-processing with examples from microbiology and immunology” by Drs. Brooke Anderson and collaborators in response to to RFA-GM-18-002: *Training Modules to Enhance the Rigor and Reproducibility of Biomedical Research*.

This submission is from Colorado State University. The proposal does not include Human Subjects, Vertebrate Animals, Biohazards, or Select Agents.

This proposal [does what]. Therefore, it would be useful if one of the reviewers had [specific expertise].

**Please assign the application to the following:**

**National Institute of General Medical Sciences (NIGMS).** *Rationale:* [Why]

We thank you for the opportunity to submit this proposal.

Regards,

Brooke Anderson (PI)

Mike Lyons (Co-I)

Marcela (Co-I)

Mercedes (Co-I)

Others?

1681 Campus Delivery

Fort Collins, Colorado 80523-1681

Telephone: 203-508-2738

Email: [brooke.anderson@colostate.edu](mailto:brooke.anderson@colostate.edu)

## Budget justification

### Personnel

**Brooke Anderson, Ph.D., Principal Investigator, *x academic person-months, x summer person-months (20% effort) in Years 01 through 02, x academic person-months, x summer person-months (5% effort) in Year 03.*** Dr. Anderson is an assistant professor of Epidemiology in the Department of Environmental & Radiological Health Sciences at Colorado State University, with an affiliate position at the Department of Statistics. She is an expert in R programming and has created and published several open-source R packages, in particular to facilitate environmental epidemiological research. She has experience creating R programs to work with large data, including climate model output and large weather datasets, as well as programs that interface with open web-based datasets. She is the co-instructor of a series of Massive Open Online Courses on *Mastering Software Development in R* through Coursera and an associated open online book. Dr. Anderson will lead the development of all training modules developed through this grant, including through supervising the development and integration of training materials from co-investigators. She will also lead user testing and other evaluation of all developed modules to ensure the developed modules are clear, effective, and well-matched to meet the needs of biological researchers from a variety of scientific backgrounds, including those new to programming.

**Mike Lyons, Ph.D., Co-Investigator, *x academic person-months, x summer person-months (5% effort) in Years 01 through 02, x academic person-months.***

**Marcela Henao-Tamayo, Ph.D., Co-Investigator, *x academic person-months, x summer person-months (5% effort) in Years 01 through 02.***

**Mercedes Gonzalez-Juarrero, Ph.D., Co-Investigator, *x academic person-months, x summer person-months (5% effort) in Years 01 through 02.***

### Travel

**Domestic travel.** Funds for PI (Dr. Anderson) to travel to one domestic conferences (\$1,500 per conference) to learn about cutting edge reproducible research techniques. Potential conferences to be attended include the International R Users' Conference (UseR) on the years it is in the U.S. (typically every other year) or the Annual RStudio Conference. This domestic travel budget also includes funds (\$900 per trip) for Dr. Anderson (PI) to travel to up to two Program Meetings over the course of the project. No travel is anticipated in Year 3 of the project, when the focus will be on final evaluation and refining of the training developed and published in Years 01 and 02.

- Year 01: \$2,400
- Year 02: \$2,400
- Year 03: \$0

### Materials and Supplies

Annual funds (\$1,000 / year) are also requested for recording equipment (e.g., microphone), screen-capture software (e.g., *Camtasia*), other software, and books to facilitate the proposed training module development.

**Conference Registrations.** Funds are budgeted for Years 01 and 02 for Dr. Anderson to register for a yearly domestic conference on cutting-edge tools and principals for conducting computationally reproducible research (e.g., UseR or RStudio Conferences). Attending a conference each year will help us include the most up-to-date tools and approaches in the developed training modules.

- Year 01: \$500
- Year 02: \$500
- Year 03: \$0

**Hospitality.** Funds are budgeted each year to provide breakfast, lunch, coffee, and snacks for two days to 20 people (for the proposed annual extended user testing meetings at Colorado State University; budgeted at \$850 / year). Colorado State University provides room reservations free to faculty for similar events, and so funds to rent a space are not required (See Letter of Support, Dr. Jac Nickoloff).

- Year 01: \$850
- Year 02: \$850
- Year 03: \$850

**Consulting?** For evaluation of the completed modules. Also, for recording demographics, etc., for evaluation purposes. Check the requirements in the grant call for this. *Check STEM contact for this.*

## Project Abstract:

We propose to develop training modules for improving the reproducibility of experimental data recording and pre-processing in scientific research. We aim to ensure these training modules are useful to laboratory-based researchers, who may have less prior training in open source software tools for reproducible research than researchers from biostatistics, epidemiology, and other disciplines. To ensure this, we will feature in these training modules examples from microbiology and immunology. We will create two sequences of modules that focus on improving computational reproducibility in the recording and pre-processing of experimental data, each containing approximately 12 modules, each featuring 5–30 minute videos, with supplemental online text, references, and practice exercises. The first sequence will be “Improving the Reproducibility of Experimental Data Recording”, and it will include modules on ... . The second sequence will be “Improving the Reproducibility of Experimental Data Pre-Processing”, and it will include modules on ... . These two sequences of training modules will be collectively published as an open online book using the *bookdown* technology. Each module will form a chapter of this book, and will feature an embedded YouTube video of 5–30 minutes, with accompanying text in the book to provide trainees with a more detailed written reference they can refer to after completing the video module. Each module’s chapter will conclude with practical exercises or open discussion questions to complement the material taught in the video. To ensure this material is completely free and open to researchers in the United States, we will publish this online book and the videos under a Creative Commons license.

## **Project Narrative:**

We will develop training modules for improving the reproducibility of experimental data recording and pre-processing in scientific research. To ensure accessibility and relevance to laboratory-based researchers, we will feature in these training modules examples from microbiology and immunology. We will create approximately 25 short training modules collected in two sequences, one focusing on reproducible approaches to recording experimental data and one on reproducible approaches to pre-processing experimental data. Each module will feature a video lecture of 5–30 minutes, and the full collection of video modules will be embedded in a free, open online book, with supplemental text and practical exercises to accompany each module. Training modules will be evaluated for researchers at a variety of training levels (undergraduates to faculty), drawing mainly from the Microbiology, Immunology, & Pathology Department of Colorado State University.

## Specific Aims

**Significance and educational aims of proposed modules.** Among the steps in conducting experimental research, the collection and pre-processing of experimental data are steps where it is critical to ensure good practices to ensure research reproducibility. However, much of the training available for computational reproducibility focuses on later steps of the research process, such as the analysis of processed experimental data. Here, we aim to develop training modules that focus on principals and techniques of improving the reproducibility of research at these stages of the research process. We will focus on making these modules accessible and useful to laboratory-based researchers by including examples of improving reproducibility at these stages of microbiology and immunology research projects and will evaluate the training modules through user testing among laboratory-based researchers.

**Proposed content of training modules.** We will develop two sequences of modules to train researchers in how and why to improve reproducibility in the collection and pre-processing of experimental data, including training on implementing these approaches using open source R software tools. Working with laboratory-based co-investigators on our team, we will ensure that these modules and the examples used in them are approachable and useful to researchers without extensive computational training, helping the modules address an audience beyond those of existing training materials on R programming tools for reproducible research. Further, the training modules will focus on reproducibility in the data collection and pre-processing stages of projects, rather than in experimental design or data analysis.

The first sequence will be “Improving the Reproducibility of Experimental Data Recording”, and it will include modules on the principals of the tidy data format, creating and using spreadsheet templates for data collection, developing project templates for organized and consistent data and meta-data collection, harnessing version control to improve transparency in data collection, and using GitLab for version-controlled collaborations. The second sequence will be “Improving the Reproducibility of Experimental Data Pre-Processing”, with modules on how and why to use code scripts for data pre-processing, creating reproducible data pre-processing protocols using *rmarkdown*, examples of developing reproducible data pre-processing protocols, and converting from complex Bioconductor data types to tidy data formats to allow use of R’s “tidy” data tools.

**Format of training modules.** Each module within each of these sequences will focus on a video lecture of 5–30 minutes. These videos will be collected together in an online book, where each module will form a chapter with an embedded video, and text and applied exercises or discussion questions will accompany each video. This book will be freely and openly published online under the Creative Commons license, to ensure it is available to any U.S. researcher. To ensure compliance with x, we will include in the online book transcripts for each training video.

**Evaluation of training modules.** We will conduct two-day user testing sessions each year of the grant. **These will be focused on scientists at a variety of levels (undergraduate to faculty) and will determine the usefulness, clarity, and relevance of the developed modules to these researchers.** These evaluation sessions will include live presentations of the lectures to be taped as modules, as well as directed work-throughs of the practical exercises included in the online book for each module. We will focus these testings on members of Colorado State University’s Department of Microbiology, Immunology, & Pathology. Following the user testing (e.g., six months–one year after), we will survey the lab head to determine which practices taught in the modules have been adapted.

**Project team.** This project will bring together experts in R programming (Anderson, Lyons), including its use to improve the computational reproducibility of health-related research, with laboratory-based academic researchers in Microbiology and Immunology (Henao-Tamayo, Gonzalez-Juarrero) who are **attuned to the needs of and barriers to improving the reproducibility of experimental data collection and pre-processing.** Our team will allow us to develop training modules that both present state-of-the-art approaches and tools to reproducibility, but do so in a way that is prioritized to be most useful and accessible to health researchers whose training has focused on laboratory-related, rather than computational, methods, and for whom existing training materials on computational reproducibility might be hard to understand or apply to their own research projects.

# Research Education Program Plan

## A Significance

“Does the proposed program address a key audience and an important aspect or important need in training in rigor and reproducibility? Is there convincing evidence in the application that the proposed program will significantly advance the stated goal of the program?”

## B Innovation

“Taking into consideration the nature of the proposed research education program, does the applicant make a strong case for this program effectively reaching an audience in need of the program’s offerings? Where appropriate, is the proposed program developing or utilizing innovative approaches and latest best practices to improve the knowledge and/or skills of the intended audience?”

These modules will teach the principals of reproducibility as well as introduce researchers to tools for implementing reproducible research workflows. The implementation portion of these modules will focus on tools from the open-source R programming language. R can be freely, quickly, and easily downloaded and installed to a user’s computer, allowing new users to get started quickly, a critical consideration for usable scientific software [1]. R has been maintained for over a decade by the R Development Core Team and works with all major computing platforms, ensuring widespread access, stability, and compatability, also critical for ease-of-use [2, 3]. R offers a well-developed environment for creating new tools that extend the core language [4] and includes ample tools for documenting research workflows [5, 6]. R’s status as the *lingua franca* of statisticians and biostatisticians means that its use in early stages of experimental data recording and pre-processing can help foster closer collaborations between laboratory-based scientists and statisticians throughout the research process. R can be scaled as the volume of data in projects grows [1], as it includes tools to interface with distributed computing platforms (e.g., *Hadoop* [7], *Spark* [8]), and its scripts can be integrated within workflow management systems (e.g., *Galaxy* [9, 10]).

## C Approach

“Does the proposed program clearly state its goals and objectives, including the audience to be reached, the content to be conveyed, and the intended outcome? Is there evidence that the program is based on a sound rationale, as well as sound educational concepts and principles? Is the plan for evaluation sound and likely to provide information on the effectiveness of the program?”

### C.1 Proposed Research Education Program Plan

“While the proposed research education program may complement ongoing research training and education occurring at the applicant institution, the proposed educational experiences must be distinct from those research training and research education programs currently receiving federal support. When research training programs are on-going in the same department, the applicant organization should clearly distinguish between the activities in the proposed research education program and the research training supported by the training program. The research education proposed must be **targeted to trainees and investigators at any level.**



State the **goals for education** and **justify the area of training** selected for module development in terms of its **relevance and potential impact** on improving the development of skills and knowledge important for conducting rigorous and reproducible research. Describe the **subject material** to be covered. Describe the **format** for the training module proposed and **justify it in terms of the education goals**. The **length** of the proposed training module should be explained in terms of **scope and depth of coverage** of the subject matter. In addition, **how the research education will be utilized by trainees or investigators** should be described—for example, a module on how to avoid confirmation bias to be taken by all beginning laboratory workers, or a module on appropriate design of animal studies to be taken immediately prior to beginning such work. Describe the **plans for piloting and evaluating the effectiveness** of the training module. Describe **plans for making the proposed training module section 508 compliant of the Rehabilitation Act** (29 U.S.C. '794 d), as amended by the Workforce Investment Act of 1998 (P.L. 105 220; see <http://www.section508.gov/> for additional information). Provide a **time-line for module development, piloting and refinement, dissemination, evaluation, and maintenance**. This timeline must propose **making the training publicly available within two years** of the award date."

### C.1.1 Educational goals of the modules

The importance of computational reproducibility of scientific research is increasingly recognized by scientists, journals, and funding agencies, with such "computationally reproducible" research requiring that all data and code for a research project be available and that this data and code can be used to regenerate study findings either by the original researcher or by other researchers [11, 12].

Every extra step of data formatting is another chance to introduce an error in the data. Therefore, by keeping research data pipelines simple—which can be more easily achieved if data is initially recorded in a format amenable to later data pre-processing, analysis, and visualization—researchers can decrease the potential for errors in the data and therefore improve the rigor and reproducibility of their research.

**Improving the Reproducibility of Experimental Data Recording** One key concept for improving the reproducibility of experimental data collection is understanding how to create and use the "tidy" data format, which enables later data analysis using R's *tidyverse* framework. The *tidyverse* framework enables powerful and user-friendly data management, processing, and analysis by combining simple tools to solve complex, multi-step problems, and this framework is enabled by ensuring those simple tools share a common interface: a "tidy" data format [13, 14, 15, 16]. Working within the R framework facilitates research that adheres to standards of reproducibility through scriptable data analysis that can easily be placed under version control [17]. Since the tools are simple and share a common interface, they are easier to learn, use, and combine than tools created in the classical R framework [13, 18, 19, 20]. This *tidyverse* framework is quickly becoming the standard taught in introductory R courses and books [21, 22, 23, 24, 19, 20] (see also Letters of Support [LOS], Kimmel, Peng), ensuring ample training resources for researchers new to programming, including books (e.g., [25, 26], some freely available online, e.g., [16]), massive open online courses (MOOCs), onsite university courses [22, 23, 24], and Software Carpentry workshops [27, 28]. Further, tools that extend the *tidyverse* have been created to enable high-quality data analysis and visualization in several domains, including text mining [29], microbiome studies [30], natural language processing [31], network analysis [32], ecology [33], and genomics [34].

RStudio allows users to create their own custom “Project” template, suited to a specific type of data analysis or software development, which can then be registered and accessed by other users [35]. While a “Project” can have any internal structure, a common structure can be enforced for a certain type of project through the creation of a new “Project” template, which defines the required subdirectories, structure, and file names of common elements that must exist in the project [35]. This template, when selected by a future user, will create a new directory with a “skeleton” structure, potentially including templated files (e.g., for metadata). Projects saved in this format can be easily put under *Git* version control in *RStudio*, which includes a pane that allows users to work under version control without learning command-line version control language and, if desired, easily connect the project with an online version of the project hosted on *GitHub*. This “project” framework has recently been encouraged by a number of researchers as a way to enable computationally reproducible research, especially for research conducted by teams [36, 37, 18], and the use of *Git* and *GitHub* has also been encouraged as a tool to enable reproducible research [38, 12, 17, 18, 39].

**Improving the Reproducibility of Experimental Data Pre-Processing.** Scriptable software tools bring key advantages compared to GUI software in terms of data pre-processing [39, 40, 41, 38], but it is critical to provide some training on the use of these tools for researchers new to programming. Expertise with a scripting language is not universal across the biomedical community, although literacy in programming is increasing in the sciences [12], and many now recommend programming as a critical skill for all biology Ph.D. students [1].

*Contrast the lack of guidance on experimental data recording for academic research with the guidelines from industry, including “Good laboratory practice”).*

### **C.1.2 Module subject material**

We propose to develop two collections of modules, **Improving the Reproducibility of Experimental Data Recording** and **Improving the Reproducibility of Experimental Data Pre-Processing**.

**Table 1:** Modules for 'Improving the Reproducibility of Experimental Data Recording'

Module title	Description of module content	Objectives (After taking the module, the trainee can ...)	Video Length	Extra educational materials
<b>Separating data recording and analysis</b>	Many biomedical laboratories currently use spreadsheets, with embedded macros, to both record and analyze experimental data. This practice impedes the transparency and reproducibility of both data recording and data analysis. In this module, we will describe this common practice and explain how it impedes the transparency and reproducibility of data recording and analysis. We will then outline alternative approaches that separate the steps of data recording and data analysis and explain how these alternative approaches can improve the reproducibility of biomedical research.	(1) Explain the difference between data recording and data analysis; (2) Understand why collecting data on spreadsheets with embedded macros impedes transparency and reproducibility; (3) List alternative approaches that separate data recording and data analysis to improve transparency and reproducibility.	15	(1) Discussion questions, including describing data recording approaches the trainee has previously used in research projects and the benefits and limitations of those approaches in terms of data transparency and reproducibility; (2) Short audio recording of two Co-Is giving their own answers to these discussion questions.
<b>Principals and power of the 'tidy' data format</b>	The 'tidy' data format was outlined in a 200[x] paper and has since quickly gained popularity among statisticians and data scientists. By consistently using this data format, researchers have found they can employ combinations of simple, generalizable tools to perform complex tasks in data processing, analysis, and visualization. However, despite the power of this format, it is not yet widely known or used among laboratory scientists when they record experimental data. In this module, we will explain what makes a dataset 'tidy', why this format is a powerful tool for reproducible research, and how use of a 'tidy' format for data collection can also improve the ease and efficiency of 'Team Science', including collaborations with statisticians.	(1) List the characteristics that make a dataset 'tidy'; (2) Describe how using a 'tidy' data format when recording experimental data can improve the transparency and reproducibility of research; (3) Outline other benefits of using a 'tidy' format when recording data.	25	(1) Quiz questions: For example datasets, correctly identify which of the 'tidy' data principals the dataset has or lacks; (2) Video giving answers and explanations for quiz questions, including showing 'tidy' versions of each example dataset; (3) Link to paper that established the 'tidy' data format.

**Table 1:** Modules for 'Improving the Reproducibility of Experimental Data Recording' (*continued*)

Module title	Description of module content	Objectives (After taking the module, the trainee can ...)	Video Length	Extra educational materials
<b>Designing templates for tidy data collection</b>	This module will move from the principals of the 'tidy' data format to the practical details of designing a 'tidy' data format to use for a specific research project. We will describe common issues that prevent real datasets from experimental research projects from following a 'tidy' format and show how they can be avoided when deciding the format in which to record experimental data. We will also provide rubrics and a checklist to help determine if a data collection template complies with a 'tidy' format.	(1) Identify characteristics that keep a dataset from following a 'tidy' format; (2) Convert data from an 'untidy' to a 'tidy' format.	20	(1) Applied exercise: Take a dataset in an 'untidy' format, identify what characteristics keep it from being 'tidy', and convert design a 'tidy' form of the data; (2) Video providing a detailed solution to the applied exercise.
<b>Example: Creating a template for data collection</b>	In this module, we will walk through an example of creating a template to collect data in a 'tidy' format for a laboratory-based research project. As an example, we will use a research project headed by one of our Co-Is on tuberculosis [more description of this project]. We will walk through the 'untidy' format initially used to collect data for this project, explain how this format differed from a 'tidy' format, and show how we changed the format to be 'tidy'. Finally, we will show examples of how the experimental data can easily be cleaned, analyzed, and visualized using reproducible tools once it is in a 'tidy' format.	(1) Understand how the principals of 'tidy' data can be applied to experimental data from a real research project; (2) Explain the advantages of using a 'tidy' data format for the example project.	15	(1) Discussion questions, including listing examples of how experimental datasets the trainee has previously worked with or is currently working with are 'untidy' and how they could be converted to a 'tidy' format; (2) Short audio recording of two Co-Is giving their own answers to these discussion questions.

**Table 1:** Modules for 'Improving the Reproducibility of Experimental Data Recording' (*continued*)

Module title	Description of module content	Objectives (After taking the module, the trainee can ...)	Video Length	Extra educational materials
<b>Power of using a single 'Project' directory for storing and tracking research project files</b>	To improve the computational reproducibility of a research project, researchers can use a single 'Project' directory to collectively store all research data (raw and pre-processed), meta-data, code for data pre-processing, and research products further along the research pipeline (e.g., paper drafts, figures, code for data analysis). In this module, we will show how all research project files can be collected and saved in a single 'Project' directory. We will explain how using this practice from the start of a research project improves the reproducibility of the projects, as well as how this practice facilitates the use of later tools to improve reproducibility, including version control. Finally, we will list some of the common components and subdirectories that are useful to include in the structure of a 'Project' directory, including subdirectories for raw and pre-processed experimental data.	(1) Describe a 'Project' directory, including common components and subdirectories; (2) List how collecting all research data and other files related to a research project in a single 'Project' directory improves the reproducibility of a research project; (3) Describe how experimental data collection can be integrated with a research 'Project' directory.	20	(1) Quiz questions: These will test the trainee's understanding of what a 'Project' directory is, what common components it may include, and the benefits of structuring research project files—including raw and pre-processed experimental data—within a single 'Project' directory from the beginning of the research project; (2) Video with detailed answers and discussion of quiz questions.
<b>Creating 'Project' templates</b>	Researchers can gain even more benefits, in terms of improving both the reproducibility and efficiency of research, by using a consistent structure for the 'Project' directories for all of the research projects for a research group. We will describe the benefits of using a consistent structure for 'Project' directories across different research projects within a research group, including how this practice can facilitate the re-use of code for pre-processing, analyzing, and visualizing data. Further, we will demonstrate how RStudio can be used to create a template of a research group's 'Project' directory structure, so a new project can be initialized with a skeleton directory that follows the 'Project' directory format established by the research group.	(1) Explain how using a consistent structure for research 'Project' directories can improve the reproducibility and efficiency of research projects within a research group; (2) Understand how RStudio can be used to create a template to use to create consistently-structured research 'Project' directories.	25	(1) Discussion questions, including descriptions of how the trainee has saved and tracked research project files for previous research projects and what barriers, if any, these practices introduced in terms of the reproducibility and efficiency of research; (2) Short audio recording of two Co-Is discussing how they have saved and tracked research project files in previous projects and what barriers to reproducibility these practices introduced.

**Table 1:** Modules for 'Improving the Reproducibility of Experimental Data Recording' (*continued*)

Module title	Description of module content	Objectives (After taking the module, the trainee can ...)	Video Length	Extra educational materials
<b>Example: Creating a 'Project' template</b>	In this module, we will walk through a real example of establishing the format for a research group's 'Project' template, creating that template using RStudio, and initializing a new research project directory using the created template. [Further description of the real research project]	(1) Create a 'Project' template in RStudio to use to initialize consistently-formatted 'Project' directories to store all files related to a research project; (2) Initialize a new 'Project' directory using this template.	15	(1) Applied exercise: We will provide a description of the components and subdirectories that a research group has decided to include in their 'Project' template. The trainee will need to use RStudio to create and save a 'Project' template that meets these specifications; (2) Video demonstrating a detailed solution to the applied exercise.
<b>Harnessing version control for transparent data collection</b>	As a research project progresses, a typical practice in many experimental research groups is to save new versions of files (e.g., 'draft1.doc', 'draft2.doc'), so that any changes can be reverted to earlier versions. However, this practice leads to an explosion of research project files, and it becomes hard to track which files represent the 'current' state of a project. Version control allows researchers to edit and change research project files in a way that allows them to identify and undo any previous changes while maintaining a single version of each file. Further, version control requires short messages describing each change made to each file, which improves the transparency and reproducibility of both the recording of experimental data and also the later steps of pre-processing, analyzing, and visualizing the data. In this module, we will explain what version control is and how it can be used in research projects. We will highlight how version control can improve the transparency and reproducibility of research. Finally, we will give examples of version control tools that are popular for research.	(1) Describe version control and what it does; (2) List how using version control improves the transparency and reproducibility of research.	10	(1) Discussion questions, including discussion of how the trainee has managed evolving research project files in previous projects and any barriers those practices introduced in conducting efficient and reproducible research; (2) Short audio recording of two Co-Is giving their own answers to these discussion questions.

**Table 1:** Modules for 'Improving the Reproducibility of Experimental Data Recording' (*continued*)

Module title	Description of module content	Objectives (After taking the module, the trainee can ...)	Video Length	Extra educational materials
<b>Using git and GitLab to enhance the reproducibility of collaborative research</b>	Once a researcher has learned to use git on their own computer for local version control, they can begin using version control platforms like GitLab and GitHub to collaborate with others in their research group while keeping the project under version control. These platforms allow the all collaborators to share a current version of a project directory (similar to Dropbox), but in a way that allows easy use of version control and that is more efficient for exploring (and, when necessary, undoing) the changes each team member has made to project files. In this module, we will describe why a research team may want to use a version control platform like GitLab to work collaboratively on a project. Further, we will show how to use git through RStudio's user-friendly interface and how to connect from a local computer to GitLab through RStudio.	(1) Explain the benefits of using a version control platform like GitLab, rather than Dropbox, to share project files for collaborative research projects, particularly in terms of increasing the transparency and reproducibility of a research project; (2) Describe the difference between git and GitLab; (3) Understand how to set up and use git through RStudio's interface; (4) Understand how to connect with GitLab through RStudio and how to use these version control and collaboration tools to improve the reproducibility of research projects.	20	(1) Applied exercise, with detailed instructions for each step: Use RStudio to initialize version control for a directory and to make several tracked changes. Create a matching GitLab repository and use RStudio to connect your local and GitLab versions of the directory. (2) Video walking trainees through a detailed solution to the exercise.



**Table 2:** Modules for ‘Improving the Reproducibility of Experimental Data Pre-Processing’

Module title	Description of module content	Objectives (After taking the module, the trainee can ...)	Video Length	Extra educational materials
<b>Principals and benefits of scripted pre-processing of experimental data</b>	The experimental data collected for biomedical research often requires pre-processing before it can be analyzed (e.g., gating of flow cytometry data, peak finding and quantification for LC / MS metabolomics data). While often proprietary, point-and-click software is available for this pre-processing, use of such software can limit the transparency and reproducibility of this pre-processing stage of the analysis, and point-and-click software is often time-consuming to use for repeated tasks over large research projects. In this module, we will explain how using scripts to apply open source software for this pre-processing step can improve the transparency, reproducibility, and transparency of research.	(1) Define pre-processing of experimental data and give some examples; (2) Describe how the use of proprietary software for pre-processing experimental data limits transparency and reproducibility; (3) Understand what an open source code script is and how it can be used as an alternative in pre-processing experimental data; (4) List some popular packages in R that can be used to pre-process biomedical experimental data.	15	(1) Discussion questions, including discussion of which steps are commonly used to pre-process experimental data in the trainee’s research area; (2) Short audio recording of two Co-Is giving their own answers to these discussion questions; (3) List of some popular R packages for pre-processing different types of biomedical experimental data.
<b>Introduction to R code scripts</b>	In this module, we will explain the difference between interactive software use and the use of code scripts, using examples from R. We will then demonstrate how to create, save, and run an R code script for a simple data cleaning task.	(1) Describe what an R code script is and how it differs from interactive coding in R; (2) Create and save an R script to perform a simple data pre-processing task; (3) Run an R script.	10	(1) Applied exercise: Given a simple example dataset and a data cleaning task, write and run an R script to perform the task. Then adapt that script to re-use it on a second, similar example dataset. Hints on useful R functions will be provided to help trainees new to the R language; (2) Video providing a detailed walk-through of a solution to the applied exercise.



**Table 2:** Modules for 'Improving the Reproducibility of Experimental Data Pre-Processing' (*continued*)

Module title	Description of module content	Objectives (After taking the module, the trainee can ...)	Video Length	Extra educational materials
<b>Principals and power of R's 'tidyverse'</b>	The R programming language now includes a collection of 'tidyverse' extension packages that enable user-friendly yet powerful work with experimental data, including pre-processing and exploratory visualizations. The principal behind the 'tidyverse' is that a collection of simple, general tools can be joined together to solve complex problems, as long as a consistent format is used for the input and output of each tool (the 'tidy' data format taught in other modules). In this module, we will explain why this 'tidyverse' system is so powerful and how it can be leveraged within biomedical research, especially for reproducibly pre-processing experimental data.	(1) Define R's 'tidyverse' system; (2) Explain how the 'tidyverse' collection of packages can be both user-friendly and powerful in solving many complex challenges in working with data; (3) Describe the difference between 'base R' and R's 'tidyverse'.	15	(1) Quiz: Questions will test the trainee's understanding of what R's 'tidyverse' is and why it is a powerful yet user-friendly tool for improving the reproducibility, transparency, and efficiency of research projects. (2) Video with detailed answers and explanations for the quiz questions; (3) Links to further free sources for learning more about the 'tidyverse' and how to use its tools.
<b>Complex data types in R and Bioconductor</b>	Raw data from many biomedical experiments, especially those that use high-throughput techniques, can be very large and complex. Because of the scale and complexity of these data, software for pre-processing the data in R often uses complex, 'untidy' data formats. These complex data formats are necessary for computational efficiency and to aid the structure of the pre-processing software, but the 'untidy' formats add a critical barrier for researchers who wish to explore and visualize the data, especially using the 'tidyverse' tools now commonly taught when introducing R to researchers. In this module, we will explain why complex data formats are often used in open source software for pre-processing experimental data. We will describe the 'list' data structure often used as a backbone for complex data structures, and well as provide tips on how to explore and extract data stored in R in this format.	(1) Explain why R software for pre-processing biomedical data often stores the data in complex, 'untidy' formats; (2) Describe the structure of R's 'list' data format; (3) Take basic steps to explore and extract data stored in R's complex, list-based structures.	15	(1) Applied exercise: We will provide example data in a complex, list-based format. The trainee will explore this data based on step-by-step instructions and will extract specified elements from the data format; (2) Video providing a detailed walk-through of completing this exercise, with explanations for specific steps.

**Table 2:** Modules for 'Improving the Reproducibility of Experimental Data Pre-Processing' (*continued*)

Module title	Description of module content	Objectives (After taking the module, the trainee can ...)	Video Length	Extra educational materials
<b>Converting from complex data types to 'tidy' data formats</b>	With the rising popularity of the 'tidyverse' collection of R tools, which require data to be in a 'tidy' format, R users have recognized that the use of complex, 'untidy' data formats can complicate reproducible code for data pre-processing, analysis, and visualization. Very recently, some researchers have developed tools (the broom and biobroom R package extensions) that can extract a 'tidy' dataset from data stored in a complex, list-based format. These tools create a clean, simple connection between the complex data formats often used in pre-processing or modeling experimental data and the 'tidy' format required to use the 'tidyverse' tools now taught in many introductory R courses. In this module, we will show trainees how to access these broom and biobroom packages. We will then demonstrate how these packages can be used to extract 'tidy' versions of pre-processed experimental data from their complex data formats, to allow user-friendly data analysis and visualization using the widely-taught general 'tidyverse' tools.	(1) Describe what the broom and biobroom R packages can do; (2) Explain why converting data from a complex format to a 'tidy' format can improve the transparency and reproducibility of a research project.	10	(1) Quiz: Trainees will be tested on their understanding of 'tidy' versus complex data formats, the difficulties introduced by complex data formats, and how data can be converted from a complex to a 'tidy' format in R; (2) Video discussing correct answers to the quiz questions; (3) Links to tutorials to find out more about using the broom and biobroom packages in R to extract 'tidy' datasets from complex data formats.
<b>Example: Converting from complex data types to 'tidy' data formats</b>	We will provide a detailed example of a case where data pre-processing in R has resulted in data in a complex, 'untidy' format, and where tools can be used to extract data in a 'tidy' format, which then can easily integrate with general R 'tidyverse' tools for data analysis and visualization. We will walk through an example of applying automated gating to flow cytometry data. We will demonstrate the complex initial format of this pre-processed data and then show trainees how a 'tidy' dataset can be extracted and used for further data analysis and visualization. This example will use real experimental data from research on the immunology of tuberculosis [more details on this project].	(1) List R package extensions that can be used to extract 'tidy' data from complex, 'untidy' R data formats; (2) Describe how these tools can be used in research projects to shift from data pre-processing to analysis and visualization of the processed data.	20	(1) Applied exercise: Trainees will be given an example dataset in a complex, 'untidy' data format in R and will be instructed in how to convert it to a 'tidy' format and then create some straightforward plots of the data based on this 'tidy' dataset; (2) Video demonstrating a detailed solution to the applied exercise.

**Table 2:** Modules for 'Improving the Reproducibility of Experimental Data Pre-Processing' (*continued*)

Module title	Description of module content	Objectives (After taking the module, the trainee can ...)	Video Length	Extra educational materials
<b>How RMarkdown documents can improve data pre-processing</b>	RMarkdown can be used to create documents that combine code and text in a 'knitted' document, and it has become a popular tool among statisticians and data scientists for improving the computational reproducibility and efficiency of their research. This tool can also be used earlier in the research process, however, to develop well-documented code to pre-process raw experimental data. In this module, we will show trainees the types of documents that can be created and run using RMarkdown. We will describe how RMarkdown is used among statisticians to improve the reproducibility, efficiency, and transparency of data analysis, as well as describe how it can be leveraged earlier in a research project to improve the reproducibility of the pre-processing of experimental data.	(1) Define RMarkdown; (2) Describe the documents that can be created using RMarkdown; (3) Explain how RMarkdown can be used to improve the reproducibility of research projects at the data pre-processing phase.	15	(1) Discussion questions: Including discussion of why RMarkdown (and similar approaches) could make data pre-processing more reproducible; (2) Short audio recording of two Co-Is giving their own answers to these discussion questions.
<b>How to create reproducible data pre-processing protocols using RMarkdown</b>	In this module, we will provide detailed instructions on how to use RMarkdown in RStudio to create documents that combine code and text. We will explain how these documents can be converted into different final file formats (PDF, HTML, Microsoft Word). We will show how an RMarkdown document describing a data pre-processing protocol can be used to efficiently apply the same data pre-processing steps to different sets of raw data.	(1) Define a data pre-processing protocol; (2) Create a document in RStudio using RMarkdown; (3) Render the document in multiple file formats; (4) Apply the document to several different datasets that follow the same format.	15	(1) Applied exercise: Trainees will be asked to create, save, and render their own RMarkdown document through RStudio; (2) Video providing a detailed walk-through of a solution to the applied exercise.

**Table 2:** Modules for 'Improving the Reproducibility of Experimental Data Pre-Processing' (*continued*)

Module title	Description of module content	Objectives (After taking the module, the trainee can ...)	Video Length	Extra educational materials
<b>Example: Creating a reproducible data pre-processing protocol</b>	We will provide an example of creating a reproducible protocol for the automated gating of flow cytometry data for a project on the immunology of tuberculosis [more details on project]. This data pre-processing protocol was created using RMarkdown and allows the efficient, transparent, and reproducible gating of flow cytometry data for all experiments in a research project. We will walk the trainees through the final pre-processing protocol, how we apply this protocol to new experimental data, and how we developed the protocol initially.	(1) Explain how a reproducible data pre-processing protocol can be integrated into a real research project; (2) Describe what is included in a data pre-processing protocol; (3) Understand how to design and implement a data pre-processing protocol to replace manual or point-and-click data pre-processing tools.	20	(1) Quiz questions: These will test the trainees' understanding of how and why we created well-documented and reproducible data pre-processing protocols for this project, as well as how this helps increase the transparency and reproducibility of the research project; (2) Short audio recording of discussion with the head of this example research project on how this reproducible data pre-processing fits into her research project and how use of this protocol differs from previous data pre-processing practices in the group.

The **Improving the Reproducibility of Experimental Data Pre-Processing** collection will include the following modules:

1. An introduction to R code scripts
2. The benefits of scripts for data pre-processing
3. Getting started with RMarkdown
4. The relationship between R code scripts and RMarkdown documents
5. Creating reproducible data pre-processing protocols using Rmarkdown
6. Example of a reproducible data pre-processing protocol: Automated gating for flow cytometry data
7. Example of a reproducible data pre-processing protocol: Measuring metabolite feature intensities for metabolomics LC/MS data
8. Complex data types in R and their use in Bioconductor packages
9. Converting from complex data types to “tidy” formats for data analysis and visualization with R’s “tidy” data tools

### C.1.3 Format for the training modules

- Online book created through the “bookdown” format, with each module as a book chapter. We can use Git Pages to host this (CSU options for web hosting?).
- Training videos embedded for each module, each 5–30 minutes. Videos will be similar to online course lectures and will be hosted using YouTube. Embedding in the book will allow users to watch videos without leaving the book’s webpage.
- Each chapter will end with exercise questions (around 10 questions, combination of discussion questions and applied exercises), as well as an embedded video with discussion of the discussion questions and a detailed walk-through of answers to applied exercises.
- Possibly host this through an online course platform like DataCamp?

**Online book.** To ensure that these training modules are easy for researchers to access, use, and reference, we will provide all training materials through an online book created with the *bookdown* framework [6] (see LOS, Xie). Through this new framework, we will be able to create a searchable online book that weaves R code into the text and that can include embedded tutorial videos, active weblinks to online references, and computationally reproducible practice examples and exercises. Further, by including R code examples as executable code, we will be able to use this online book to frequently check tutorial code examples to quickly identify and fix any broken tutorial code [6]. Dr. Anderson (PI) has previously created two *bookdown*-based books, *R Programming for Research* and *Mastering Software Development in R*.

#### C.1.4 Piloting and evaluating effectiveness of training modules

#### C.1.5 Insuring compliance with Rehabilitation Act

### C.2 Team

#### C.2.1 Program Director/Principal Investigator

“Is the PD/PI capable of providing both administrative and scientific leadership to the development and implementation of the proposed program? Is there evidence that an appropriate level of effort will be devoted by the program leadership to ensure the program’s intended goal is accomplished? If the project is collaborative or multi-PD/PI, do the investigators have complementary and integrated expertise; are their leadership approach, governance and organizational structure appropriate for the project?”

“Describe **arrangements for administration** of the program. Provide evidence that the Program Director/Principal Investigator is actively engaged in research and/or teaching in an area related to the mission of NIH, and can **organize, administer, monitor, and evaluate the research education program**. For programs proposing multiple PDs/PIs, describe the complementary and integrated expertise of the PDs/PIs; their leadership approach, and governance appropriate for the planned project.”

#### C.2.2 Other members of the team

### C.3 Institutional Environment and Commitment

“Describe the institutional environment, reiterating the **availability of facilities and educational resources** (described separately under Facilities & Other Resources), that can contribute to the planned Research Education Program. Evidence of institutional commitment to the research educational program is required. A **letter of institutional commitment** must be attached as part of Letters of Support (see below). Appropriate institutional commitment should include the provision of adequate staff, facilities, and educational resources that can contribute to the planned research education program.”

### C.4 Evaluation Plan

“Applications must include a plan for evaluating the activities supported by the award in terms of their **frequency of use** and their **usefulness**. The use of **multiple evaluation approaches** is highly encouraged as is **testing several groups with different characteristics**. The application must specify **baseline metrics (e.g., numbers, educational levels, and demographic characteristics of test group)** in a structured format, as well as **measures to gauge the short and long-term success of the research education award in achieving its objectives**. Applicants are expected to **obtain feedback from test group** to help identify weaknesses and to provide suggestions for improvements, and **make the evaluation and feedback data** available to NIGMS staff.”

**Learning objectives** These are what we're trying to determine were achieved by the training modules.

**Pilot / text group evaluation:**

- Work with GAUSSI to use some students as pilot testers?
- Recruit researchers / faculty as pilot testers?
- Work with CSU's Research Ethics group to figure out ways to pilot?

The key goal of this project is to develop tools that are easy to use by a broad range of applied metabolomics researchers. We will therefore conduct regular short (two hours) user testings several times per year and one long (two days) user testing session per year. The user testing groups will consist primarily of student trainees involved in applied metabolomics research from a range of departments at Colorado State University (see LOS, Clark, De Long, Heuberger). The shorter testing sessions will be used to test stable versions of the developed R packages immediately before they are published to the Comprehensive R Archive Network (CRAN). These testing sessions will ask participants to work through package tutorial vignettes and other test cases and will focus on identifying aspects of the package that cause unwanted behavior on certain computer systems or when users provide unexpected input. Further, these shorter testing sessions will be used to identify sections of vignette tutorials or help files that are unclear to targeted users. The longer, two-day testing sessions will be more open and will provide participants with open-ended metabolomics data analysis challenges, using data from *Metabolomics Workbench* and the *National Metabolomics Data Repository* that differ from the data used to develop the tools. Participants will be scheduled into groups, allowing them to participate during the two days while meeting outside obligations like classes and meetings. Participants will be encouraged to use both the tools we develop here, as well as any other available R tools, to complete these challenges in groups in a "hackathon"-style structure. Participants will be given guidance on how to use GitHub to work in groups and share final results from the challenge, a framework Dr. Anderson has successfully used in a previous similar event at Colorado State University (Figure 1). This longer testing will help us identify limitations in the usability of the tools we will develop here, validate the tools using separate data, scope future development aims by identifying analysis tools that users would have liked to have to help with these open-ended challenges but that were not yet available in the R environment, and compare the tools we develop to existing metabolomics data analysis and visualization tools. Dr. Anderson (PI) has run several two-hour user testing sessions with students from various departments of Colorado State University prior to releasing R software packages [? ?]. Further, in April 2016, she led a longer, two-day user testing session through a Weather Data Hackathon at Colorado State University (Figure 1). Around 15 people participated, including undergraduate students, graduate students, postdoctoral fellows, and professors from CSU's Departments of Atmospheric Sciences, Civil & Environmental Engineering, Microbiology, and Statistics. Some of the ideas and code developed during this Hackathon have since led to development and publication of open source software [? ?].

**Long-term evaluation:**

- Google Analytics for online book. How often are people accessing the book? How long are they spending on the book website? Where are the people accessing the book?
- YouTube analytics for the embedded videos. How often are people accessing the book? How long are they spending on the book website? Where are the people accessing the book?





**Figure 1:** Some of the approximately 15 undergraduate students, graduate students, postdoctoral fellows, and professors who participated in a two-day Weather Data Hackathon at Colorado State University in April 2016.

- Quiz for each chapter of the book? Use to evaluate how well they've mastered the material? (Possibly could use embedded Shiny apps for this? Other ways to do this?)
- Rating options for each chapter of the online book? Usefulness? What they learned?
- Survey within each chapter of the online book? Educational level, demographic characteristics.

## C.5 Dissemination Plan

"A specific plan must be provided to disseminate the finished training modules **nationally** and make them **freely accessible**. In addition, links to these modules will be posted and maintained on the NIGMS web site."

We will create an online tutorial book, since providing tutorials, example code, and example datasets can substantially improve the ability of new users to learn software tools [1]. We will use GitHub's free "Pages" web publishing framework to publish the book freely online, and we will also submit it to the *bookdown.org* website under a Creative Commons license. Dr. Anderson (PI) has previously created two *bookdown*-based books, *R Programming for Research* and *Mastering Software Development in R*. Both are publicly and freely available online under the Creative Commons license (see LOS, Xie).

We will publish the video lectures using the YouTube platform and embed these videos within the online book. The videos, like the book, will be published under a Creative Commons license.

## C.6 Timeline

"Provide a timeline for **module development, piloting and refinement, dissemination, evaluation, and maintenance**. This timeline must propose making the training publicly available within two years of the award date."



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## E Environment

“Will the scientific and educational environment of the proposed program contribute to its intended goals? Is there a plan to take advantage of this environment to enhance the educational value of the program? Is there tangible evidence of institutional commitment? Where appropriate, is there evidence of collaboration and buy-in among participating programs, departments, and institutions?”

- Computers. Access to needed software. Computer services (IT).
- Library. Access to many recent books online.
- Teaching expertise?
- Research Rigor & Ethics center / training?
- Tech Transfer
- Participating departments (and their commitment)

**Video Studio and Editing Bays.** CSU’s Morgan Library has a video studio and editing bays that can be used by anyone affiliated with CSU to record and edit video content (<https://lib.colostate.edu/technology/video-studio-editing-bays/>). These can be reserved and used for free for up to three hours at a time. This facility includes microphones, video lights, video recording equipment, and video editing software.

**Computer Assisted Teaching Support (CATS) Laboratory.** Staff and facilities for professional video recording and editing. *If we need a cost share for this proposal, their contribution could potentially be in-kind.*