

# McNeil Group Handbook

## *Policies, Procedures, and Guidelines*

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<http://mcneilgroup.chem.lsa.umich.edu/>

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# Introduction

Welcome! (Please schedule an onboarding session with me before you get started.)

## Core Values

Everyone - regardless of race, ethnicity, gender, sexuality, age, nationality, religion, ability, or socioeconomic status - is welcomed, valued, and respected within our group. We believe that everyone has something unique to contribute to the group.

We will celebrate successes, and at the same time, we will recognize that we are all here to learn and learning involves making mistakes. We aim to separate the mistakes from the people making them and to collectively learn from them.

We value teamwork and collaboration. The quality of the science we produce is more important than the quantity of results. We aim to use our time, resources, and skills to perform research with integrity and to benefit society. We also value teaching, mentoring, and outreach activities aimed at encouraging the next generation of scientists to be successful.

Respectful dialogue is expected at all times. We feel empowered to speak up when a community member isn't upholding these core values. We are all here to learn, grow, thrive, and support each other.

## Your Health & Well-Being

(Adapted with permission from [Jen Heemstra](#))

### Philosophy

We are all here to grow as scientists by pursuing ambitious research goals. However, this goal should not come at the cost of your health and well-being. Your mental and physical health are the most important consideration. You are more likely to be successful if you take care of yourself. Below are some general guidelines but every situation is unique, and Anne is always open to discussion, so don't hesitate to ask.

### Mental and physical health concerns

If you are not feeling well, please seek out help immediately. If you have an acute situation, take the day off with no questions asked. Just give Anne a heads up so that she knows you are okay - it is sufficient to Slack and say that you have a "personal health emergency." If you need to take more than a day off, you can work with Anne (and the department) to facilitate

this absence. Being an undergraduate, grad student, or postdoc is stressful. We all care about you and are here to support you - just let us know how we can help.

- For help contact: **Counseling and Psychological Services (CAPS)** at (734)764-8312 or the **University Health Service (UHS)** at (734)764-8320. For confidential support related to sexual assault call (734)936-3333.

## Personal emergencies

In these situations, the top priority is taking care of yourself and dealing with the situation. Communicate with Anne to let her know that you are dealing with something and approximately how much time you expect to be absent.

## Work-life integration

I want you to push your limits to explore what you are capable of. The key is to know when to give yourself a break or some time off. Similar to playing sports, you advance by pushing out of your comfort zone, but if you push too hard you end up injured and stuck on the sidelines. Managing your motivation and work habits while integrating interests and commitments outside of work is a key self-leadership skill that will serve you well throughout your career, and now is a great time to build that skill.

# Group Policies

## Group collaborations

Collaborations are a vital part of the scientific enterprise. McNeil Group members are encouraged to participate in both external collaborations (within and/or outside of the Michigan) as well as internal collaborations (group members working together on related projects). There are many benefits to these collaborations. Oftentimes, the project's timeline can be expedited when multiple people are working together. In addition, your collaborators can give research projects added areas of expertise and new directions.

When you agree to engage in a collaborative project, you are committing to providing the collaborator with the highest possible quality of materials/data and in the fastest time possible. The group policy is that with each sample you must provide the collaborators with the notebook pages that correspond to the experiments, and accessible copies of all relevant data (e.g., <sup>1</sup>H NMR or IR/Raman spectra, SEM or adsorption data, elemental analysis, etc.). It is imperative that all lab members conform to the above criteria to ensure a productive collaboration. Also, you should cc Anne on ALL communications with collaborators, no matter how small the detail or communication.

## Coauthorship policies

Anyone who wants to earn coauthorship on another student's project must discuss it with Anne and the lead author before doing the work. To earn coauthorship, one should make significant intellectual and/or experimental contributions to a paper.

For intellectual contributions, the coauthor should make suggestions that impact the research directions throughout the entirety of the project, beyond group meetings, subgroup discussions, and informal conversations in the lab. They should be continuously and actively reading papers in the field, helping analyze and discuss research results on a weekly basis, and helping make decisions that impact project direction.

For experimental contributions, the coauthor should contribute meaningful data that impacts the conclusions of the work. It should involve a significant amount of the researcher's time (e.g., more than 1 week) and the data should impact the conclusions of the work. As an example, co-authorship is warranted if the experimental contributions appear in a figure in the manuscript.

All other forms of assistance (e.g., helping collect field samples, taking a few spectra, running some samples on a technique you are already trained on that doesn't take too long) should be acknowledged but not rise to the level of coauthorship.

Note that high school students, undergraduate students, and rotation students can earn co-authorship with less significant (but still meaningful) contributions (e.g., providing data that appears in the SI only) due to their more limited time in the lab.

## Research group meetings

Research group meetings occur every week. (See the McNeil Group "Shared Drive" Group Meeting Schedule folder for the schedule.)

Each member of the presenting subgroup has 30 min to present something that they want to discuss. Students should think carefully about how to use this time. Do you want us to help you troubleshoot an experiment? Do you need help with planning what experiments to do next? Do you want a second opinion on your data analysis and interpretation? Do you think your project should switch directions?

Then the student should craft a short (but polished) slide presentation with all necessary information to accomplish their goal. A few general guidelines: All experiments should be accompanied by the notebook page and with a chemdraw scheme and literature references. All data should be processed as if publishing it (do not post raw data) and the analysis should be clearly depicted using ChemDraw and Illustrator/Photoshop.

In addition, each week 2-3 students will have an individual meeting with Anne. Once or twice a year, the group will go off-site for a retreat where everyone will give a formal research presentation.

### Public presentations of research

All forms of public research presentations, whether conference talks, posters, or published papers are a reflection of the entire research group and *therefore must be approved by Anne at least 2 days in advance of their presentation.*

### Rotation students

Rotation students should plan to work *at least* 20 hrs per week in the lab. At the end of the semester, rotation students will present a 30 min formal presentation on their work to the group.

### Undergraduate researchers

All undergraduates are expected to work 3 h/credit-hour and can only perform research if a graduate student or post-doc is also in the lab. The undergraduates are expected to attend and participate in all group meetings.

### AI usage in your research

If using generative AI tools, please use the UM GPT if you are entering information that would reveal your original research ideas (i.e., to avoid being scooped).

### Gateway/Theses/Papers/Research Statements

Permissible is edits to your own writing (e.g., grammar and spelling). If Grammarly is used for editing your text, just acknowledge its use. If you are uploading an entire document to Grammarly for large-scale changes, share the first draft and final draft with Anne.

Not permissible is using AI tools to draft/generate content (e.g., paragraphs, sentences) from scratch. Also not permissible is asking AI tools to find references for sentences.

Any substantial use (outside of language improvement, grammar correction, and readability enhancement) of AI during manuscript preparation must be transparently disclosed in the Acknowledgments or Methodology section.

### Figures that contain research data

Cannot be used for creating, manipulating, generating original research figures and images.

### Non-data schemes within papers (adapted from ACS journal policy)

The use of AI tools for text or image generation should be disclosed in the manuscript within the Acknowledgments section with a description of when and how the tools were used. For more substantial uses, authors should provide full details within the Methods or other

appropriate section of the manuscript. For graphics, a brief description of AI use should be included in the figure caption to explain to readers how the image was created.

AI-generated images should not be used within Table of Contents (ToC) graphics, as they do not have captions immediately adjacent to the image where the use of AI can be transparently explained. The use of AI tools for image generation in cover artwork is permitted but should be disclosed in the cover art caption submitted alongside the artwork file.

#### **Non-data schemes within presentations (subgroup, individual, internal/external)**

Gen AI tools can be used to generate smaller components of larger images (e.g., a specific flask) but the compilation of the larger image and idea for the image came from you (the scientist). Also, you must properly cite the AI tools used and clearly explain how it was used.

#### **Doing research itself**

Cannot be used for creating original research data

#### **Writing code**

You can only use AI to generate code IF you know how to read, edit, and interpret the code that is generated.

#### **Peer review (adapted from ACS journal policy)**

Uploading unpublished manuscripts, peer review reports, or editorial communications into public AI platforms violates confidentiality and ethical guidelines. Peer reviewers are strictly prohibited from using generative AI to evaluate manuscripts or write review reports. Disclosing any part of the submission or the peer review report itself to a text generation service (or any other third-party tool) is a breach of this confidentiality, and thus a violation of the ACS Ethical Guidelines.

### **Data Storage: McNeil Group Shared Drive**

After joining the group you should set up some space on the McNeil Group “Shared Drive” to store publishable data, publications, presentations, and gateway- and thesis-related documents. Please create separate sub-folders for “processed data”, “presentations”, “publications”, “candidacy”, and “thesis”.

### **Slack**

Slack is a cloud-based app that we use for all group communication. All students should join our Slack team “McNeil Group” when you start. Channels should be used to send messages to large groups of people. Slack can also be used to send direct (private) messages to anyone in the group, including Anne. Slack should be used for all file sharing as well, you can upload/download, share via Google drive, etc. One really nice feature of Slack is that both the files and messages are text searchable.



# Sustainability Initiatives & Policies

## Disposable versus reusable lab supplies

Because our lab cares about carrying out our research using the most sustainable practices, we will aim to use exclusively reusable lab supplies (where practical). For example, our lab will only use reusable glass syringes and metal needles unless our chemistry requires a disposable syringe (e.g., PFAS work). Our lab will wash test tubes after chromatography columns. Best practice would be to recover the solvent from the rotovap trap and use that for the first wash of the test tubes.

## Reusing 4L solvent bottles for liquid hazardous waste

Our lab participates in a campus-wide initiative to reuse 4L solvent bottles for liquid hazardous waste. Once the bottle is empty, deface the label and place it under the hood (in the lab's central storage area) for storage. When you need a waste bottle, grab one from the storage and grab a waste sticker from the department hall waste closet and add it to the bottle.

## Composting

In each lab, there is a small compost bin to place paper towels that were used to dry clean hands. In the kitchen, there is another small compost bin for food waste. Both types of bins must be emptied by the students into the larger hallway compost bins.

## Recycling styrofoam

The group member who opens packages needs to sort the foam (peanuts versus rigid foam) into two separate clear, plastic bags. Once full, they should be brought down to the loading dock and placed in the appropriate gondola.

## Oven timers to reduce energy consumption

To reduce energy consumption of laboratory equipment, we placed our drying ovens on timers that automatically turn them off at 7 pm and back on at 7 am. In addition, we maintain our oven temperatures to 120 °C to minimize heating/cooling times and energy consumption.

## Other recycling initiatives

The 2nd floor in the '88 building has a recycling center for writing utensils (markers/caps, pens/caps, permanent markers/caps, mechanical pencils, wooden pencils, and highlighters), batteries, electronic media, colored caps, white caps, pipette tip boxes, and ice packs.

# Advice

## Resources on campus

The [Rackham Graduate Student Emergency Fund](#) is intended to help meet the financial needs of Rackham graduate students who encounter an emergency situation or one-time, unusual, or unforeseen expenses during their degree program.

The [Rackham Postdoctoral Fellows Emergency Fund](#) is intended to help meet the financial needs of postdocs who encounter an emergency situation or one-time, unusual, or unforeseen expenses.

For U-M students, staff, faculty, and surrounding community, the [Center for Education of Women+](#) offers opportunities for scholarships, emergency grants, sponsorships, fellowships, and more for a range of situations and life circumstances.

If you or someone you know is feeling overwhelmed, depressed, and/or in need of support, several services are available. Contact [Counseling and Psychological Services](#) (CAPS) or email: [caps-uofm@umich.edu](mailto:caps-uofm@umich.edu). You may also consult [University Health Service](#) for other health needs and [for alcohol or drug concerns](#).

Title IX prohibits discrimination on the basis of sex, which includes sexual misconduct — including harassment, domestic and dating violence, sexual assault, and stalking.

I encourage anyone dealing with sexual misconduct to talk to someone about their experience, so they can get the support they need. Confidential support and academic advocacy can be found with the [Sexual Assault Prevention and Awareness Center](#) (SAPAC) on their 24-hour crisis line, (734)936-3333. Such violations can also be non-confidentially reported to the [Office for Institutional Equity](#).

## Grad school (and postdoc) skills development

Here we suggest some year-specific goals for graduate students because it is oftentimes difficult to assess your progress because there are few concrete milestones in graduate school. It's easy to feel like an imposter when you don't know how to assess yourself. (Special thanks to Jessica Tami for leading this group discussion in Feb 2022.)

### Year 1

Learn to effectively search through the literature to answer specific questions and keep up-to-date with the latest science in your field. Some resources to use are: Reaxys, SciFinder,

Web of Science, Google Scholar, and checking ASAPs of the journals you read. Read as much as you can. This guideline is true for every year of graduate school and beyond.

Learn to extract the important information from papers efficiently. Start by reading introductions to situate yourself in your field and understand what has been done previously. Then read the abstracts and conclusions. Then incorporate results and discussion. Eventually, with a lot of practice, you will look at figures and understand the novelty or improvement of methods without having to read the entire paper. Try paraphrasing published work to improve on your scientific writing. How would you phrase the introduction? How would you conclude the paper?

Build self confidence and comfort with relevant lab techniques, lab equipment, and instruments. This comes with practice! We also have manuals for all of our instruments in case you forget something.

Attend seminars (aim for 1 per week) and be engaged. Read a paper by the speaker before attending. In addition, pay attention to the speaker's presentation skills and aesthetics so you can learn how to present *your* research most effectively. If you learn one thing (even if it isn't science) at a seminar, it was worth your time.

Apply to fellowships! There are a lot of fellowships for 1st and 2nd year graduate students (NSF, NDSEG). You will understand your project in a deeper way and get practice with scientific writing.

THIS IS YOUR TIME TO MAKE MISTAKES! If you make a mistake, it is not the end of the world. You will learn and probably never make the mistake again. Please do not be afraid to ask questions. It's better to ask and do something correctly than say nothing and potentially hurt yourself. Your first year is all about learning, learning, learning. Not producing, producing, producing.

## Year 2

Practice public speaking. Explain your project to a variety of people. How would you tell your parents about your science? Your younger sibling? A tenured professor in your field? An assistant professor in another department? Internal symposia (Karle, Macro, etc.) are good opportunities to practice your speaking skills. Participate in all relevant ones.

Ask yourself about the *what*, *how*, and *why*'s. What do reagents do in your reaction flask? What is the mechanism? Why are you using this number of equivalents? How will I purify the crude reaction mixture? Thinking ahead will help you answer questions during group meetings, subgroups, and your gateway exam.

Know your basics from classwork and how they apply to your project. Learn how to answer questions eloquently and make educated guesses and hypotheses on the spot. This is a

follow-up to point #2. You will not always know every answer to every question but when you know the basics of your project, you can generally guide yourself to the answer.

Continue attending seminars. Start building the confidence to ask the speaker any questions you might have.

This needs to be reiterated: read, read, read!

Continue applying to fellowships if you are still eligible!

Draw writing inspiration from papers that do similar science to your project. Start writing an intro to your first paper. This exercise will help you see gaps in your own project and knowledge. Don't be afraid to put words on paper, your first draft will never be your final product. Just get started!

### Year 3

Start thinking about your future career and explore different career paths. Attend career workshops and give informational interviews. Start networking with people who have this career, as their advice and support will be really helpful. McNeil Group alumni, LinkedIn, and DiversifyChemistry are good sources for finding people to interview.

Attend different professional development activities. The university and department put on a lot of events for resume building, public speaking, scientific writing, etc.

Continue attending seminars and reading the literature!

Attend an external conference (ACS) and present your work.

Get involved with grant-writing, paper-writing, and/or helping write a Perspective or Review article.

Mentor an undergraduate or a rotation student.

### Year 4

Go to job recruitment sessions to start preparing for future job searches. Network with professionals who work in industry, government, academia, etc.

Mentor an undergraduate or a junior graduate student.

Continue attending seminars and reading the literature!

Attend a more specialized external conference (Gordon, etc.) and present your work.

Get involved with grant-writing, paper-writing, and/or helping write a Perspective or Review article.

Start planning your thesis chapters and consider adding a new project and/or starting a collaboration.

## Year 5

Start applying for jobs and/or postdoc positions in early Fall.

Start writing your thesis. Whenever you think you should start writing, start a month earlier! It takes longer than you think AND it is due to your committee 14 business days before your defense.

Mentor an undergraduate or a junior graduate student.

Continue attending seminars, conferences, and reading the literature!

Get involved with grant-writing, paper-writing, and/or helping write a Perspective or Review article.

## Post-docs

Don't be afraid to try *new* things! You are supposed to *grow* a ton during your postdoc time so look for opportunities to develop new skills and research directions.

Consider applying to different jobs (industry, academia, government, non-profits, etc) to see which feels right. Reassessing your goals is OKAY! Do what is best for you.

Practice for the job that you want. If you want to be a professor, ask to teach a class. Ask to meet with seminar speakers when they come through Michigan. If you want to go to industry, try to get involved with collaborations with other groups and manage those collaborations so that productive scholarship results.

Be efficient with experimental designs and your time.

Mentor an undergraduate or a junior graduate student.

Continue attending seminars, conferences, and reading the literature!

Get involved with grant-writing, paper-writing, and/or helping write a Perspective or Review article.

## Advice for Running Reactions

For a great reference on synthesis and lab techniques, check out the “Not Voodoo” website by Alison Frontier (University of Rochester) at <http://chem.chem.rochester.edu/~nvd/>. See also, “The Laboratory Companion” by Gary S. Coyne and John S. Wiley and “Advanced Practical Organic Chemistry” by J. Leonard, B. Lygo, and G. Procter.

Start with pure reagents and chemicals. See “Purification of Laboratory Chemicals” by Armarego and Chai for detailed information on how to purify common reagents and solvents. Garbage In = Garbage Out!

Run reactions on a small scale the first time (~100 mg or less!). After you have worked out the reaction conditions and purification procedure you can scale up. Do not scale up a reaction more than 3-fold of your previous successful attempt. Monitor your reactions by TLC. You can supplement TLC with GC analysis, crude NMR spectra, and IR. None of these techniques are a substitute for TLC. Take the time to identify by-products the first time through a synthesis.

Always work up reactions immediately upon completion.

## Searching and reading the literature

### Searching the past literature

#### Reaxys & SciFinder Scholar

Excellent resources when searching for specific chemical reactions & conditions.

#### ISI Web of Science

There are several very useful functions of this website.

**Cited References Search:** Use this search to find all articles that cite a key paper. This search is especially useful because you can also find articles that cite the paper that cited your key paper!

**General Topic Search:** Use the “and” command to link two concepts and use “\*” to expand. For example, if you want to search for microplastics, but also want to include any search where “microplastic” is also used. Your search command would read “microplastic\*”

**Author Search:** Use this search to find all articles published by an author. You can then refine this search using keywords, dates, or document type, etc.

Note that both search engines allow you to refine your results by narrowing the list and by analyzing the list. For example, if you are searching for a starting material, you can refine your SciFinder result list by “commercial availability.” Or if you are searching for articles with a name like John Smith, you can refine by first analyzing the “institution type” and then only select those articles by John Smith at University of Michigan. Other useful tools include Wikipedia, Google, Google Scholar, “Comprehensive Organic Transformations” by Larock, and eROS (encyclopedia of reagents for organic synthesis.)

### Google

This search engine can provide a useful starting point for any literature search.

## Reading the Current Literature

You should aim to read one new paper each day of the week. Keeping up with the current literature is essential to becoming a creative, independent, and successful scientist. You should aim to gain breadth (by reading newly published papers *outside your project area*) and depth (by reading newly published papers *in your project area*). Balance your reading between breadth and depth. To set yourself up for success, here are some strategies and tips from group members on how to identify papers to read.

### Research App

Receive content from specific journals, or create keyword (or author or topic) searches and have papers delivered in a newsfeed type style to your device (similar to RSS feeders). Read, bookmark, or save for later.

### Publication Alerts

**Google Scholar** You can set alerts for specific authors or keywords.

**ACS Journals** You can sign up to receive alerts for new papers published in specific journals, or set alerts for specific keywords in newly published papers in ACS journals, or set an alert for when specific publications have been cited.

**SciFinder Scholar (or Web of Science)** You can set alerts for papers published with specific keywords and set a frequency of emails.

### Other Tips

As you identify papers to read, assign them to a specific day so that you always have a paper on deck and are not spending time looking for something to read each day. Then prioritize reading that designated paper for that day first thing in the morning, when you arrive at work. When deciding whether you want to add a paper to your “deck”, read the title, then abstract, then scan the figures. If you are still interested to know more, add it to your reading list.

# Expectations in the lab

## Work Expectations

Your success in graduate school is not correlated with the number of hr/wk that you work, but how well you use the time you have. Just physically being in the lab is not enough, you need to focus your time and effort when in the lab on experiments (and readings) that move the project forward.

A good general guideline is that the “front edge” of your project (which is the **THING** you are stuck on) should move forward EVERY day. To accomplish this task, you should set daily research (and learning) goals that focus on that “front edge.” What is holding back your next paper? Then check in with those goals at the end of EVERY day. Some goals should be experiment-based, but some goals should also involve reading the literature to learn more about an important aspect of your project.

Try to avoid being in a materials- or equipment-limited world. You should get into the habit of planning far enough ahead so that you don’t have to wait for a chemical or piece of equipment to arrive. Similarly, bringing up starting materials should not be a daily goal, rather it should be happening in the background. Your daily goals should always include key experiments where the results intellectually move the project forward.

Weekly goals can also be helpful, along with monthly goals, although keep in mind that these are more projections than goals, and they may change as new results are acquired. Frequent “research direction” meetings with Anne can also be helpful, especially when unexpected results throw a wrench into your weekly or monthly plan.

Other really useful tips and strategies to monitor “how well” you are doing can be found in the self-evaluation document on our group website. By the time you graduate, you should be able to answer “yes” (or equiv) to all the questions in that document. The self-eval can serve as a great “to-do” list for your own professional growth.

**Vacations:** Each graduate student/postdoc is allotted 20 days (starting Jan 1, 2027) of vacation per calendar year (Jan-Dec). This number is inclusive of all UM-recognized holidays. Note that sick days do NOT count as a vacation day. If you join the lab mid-year, the number of vacation days will be prorated based on the start date. To keep track of everyone's dates, there is a shared Google calendar. You should write your initials on the date(s) you will be taking off AND what vacation day that is for you (e.g., 10/20 2027). Vacation days can roll over into the next calendar year.

# Lab safety

## General

Make sure you complete the UM-OSHA Comprehensive Laboratory Safety Training course. Upload a copy of your completion certificate to the McNeil Group “Shared Drive” Safety Folder prior to starting lab work.

Make sure you read and sign all lab-relevant SOPs (binder in kitchen).

Make sure that you complete the safety checklist (next page) and send a signed copy (PDF) to Anne before beginning research. Upload a copy onto the McNeil Group “Shared Drive” Safety Folder as well.

Notify the group safety officers AND Anne immediately if you have been injured or spilled a toxic, caustic, or flammable compound.

Lab coats and safety glasses must be worn when doing work, either at your bench, hood, or sink OR if you are talking/standing next to someone who is working at the bench, hood, or sink. If you see someone working without a lab coat and/or safety glasses, please remind them of the appropriate personal protective equipment needed for working in the lab. If the problem persists, please notify Anne.

Open-toed shoes and shorts/skirts (without leggings) cannot be worn in the lab.

Headphones (even single-ear wearing) are not allowed in the lab.

Notify group members when you are leaving for the night. This habit helps to ensure that nobody is working alone!

## Guidelines for a Safe Working Area

### Bench and Hood Area

Your workspace should not be cluttered. You must be able to place a new vial/flask/beaker on your bench. All reagent and solution bottles must be clearly labeled without use of chemical abbreviations.

Nothing can be hanging off the edge of benches or shelves. Flammable solvents and reagents cannot be located within 18” of the ceiling.

No objects can be within the back 4" of your hood unless it is on a shelf. Check that all water, air and N<sub>2</sub> lines are secured with copper wire. Ensure all tubing and power cords are free of defects.

All chemical waste must be clearly labeled with no chemical abbreviations and dated. Chemical waste should be capped when not in use. Glass containers containing chemical waste within 4' of a drain must be in a secondary container.

### Instrument room and shared spaces

If you are responsible for an instrument that generates chemical waste, ensure that the waste bottle is properly labeled, dated, placed in a secondary container and has an appropriate cap.

Claim any chemicals left in the balance area and return them to the proper place.

### **Emergencies**

Call the Department of Public Safety by dialing **911** from a campus phone or **734-763-1131** from a cell phone. Call **Chris Peters** (Departmental Lab Safety) at **734-763-4527** or [chrpeter@umich.edu](mailto:chrpeter@umich.edu) or **Tracy Stevenson** (Departmental Lab Safety) at **734-764-7316** or [steventi@umich.edu](mailto:steventi@umich.edu).

## Lab entry - safety checklist

*Please complete this checklist with your mentor and the group safety officer, and send Anne a signed copy as a pdf file as well as upload a copy into the "safety" folder in Drive before beginning to work in the lab.*

| <b>Student</b> | <b>Mentor</b> | <b>Task</b>                                                                                                                                                                                                                           |
|----------------|---------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|                |               | I have completed the online OSHA safety training and uploaded my certificate on Drive.                                                                                                                                                |
|                |               | I have read the University of Michigan chemical hygiene plan and the group-specific hygiene plan, and have read and signed all SOPs.                                                                                                  |
|                |               | I have received safety glasses and a lab coat and agree to wear them at all times when in the lab.                                                                                                                                    |
|                |               | I have completed a safety walk-through with the group safety officer.                                                                                                                                                                 |
|                |               | I know how to access MSDS (material safety data sheets), and I will refer to these if I have any questions.                                                                                                                           |
|                |               | I am aware of emergency phone numbers and department contact numbers in the event of an accident, chemical spill, or other emergency.                                                                                                 |
|                |               | I will seek advice from experienced group members about all new procedures, and I will consult with Anne if any procedure poses a potential safety concern.                                                                           |
|                |               | I will maintain a safe and clean work environment, will properly label and dispose of hazardous materials, and will safely store and handle all chemical reagents.                                                                    |
|                |               | I have discussed with my mentor how to properly handle and label chemical waste (solid & liquid) related to my research.                                                                                                              |
|                |               | I will conduct my research with honesty and integrity and will not intentionally fabricate or misrepresent any scientific data.                                                                                                       |
|                |               | I will consult with Anne on any issue that poses a safety concern. If I see an unsafe operation being conducted, I will ask the coworker to correct the problem, and I will consult with Anne if the problem persists or is repeated. |
|                |               | I have read the entire group manual and understand what is expected of me. I am aware of the lab protocols for keeping complete and accurate records of my research.                                                                  |

## Lab notebook (OneNote) guidelines

### Philosophy

Your notebook is an electronic record that must document in sufficient detail your research process & the data collected (more details on expectations below). Your notebook forms the basis of your published work. It is a legal document that is used in patent applications and to defend against research misconduct. It belongs to UM, not you.

### General guidelines for everyone

Every experiment you do must be recorded in the lab notebook. The best practice is to update your notebook at the end of each day so that you capture as much information as accurately as possible. Taking the time to update your notebook each day also helps you process what happened, and plan your next experiments. The group policy is that any new experiments must be added to your notebook within one week of performing it...at the latest!

DO NOT ERASE or DELETE anything once it has been added. Instead, use a strike-through and add a comment about what has changed and why it has changed. All edits to your notebook are tracked and provide an audit trail of your work. Honesty is the best approach and it helps us trust one another.

Ask Anne to share the lab notebook with you. Then create a new “notebook” section for yourself and then create sub-sections for each project you have or based on your year in the program. Assign each notebook a different number. Each notebook should have as its first page a graphical TOC with hyperlinks to the experiment pages. Experiment pages within the notebook should include your initials—notebook number—page number.

All data, even outliers, must go in the electronic notebook as “raw data.” If the processed data is missing some of the raw data, you must explicitly say why and provide statistical grounding or other evidence for why that data can be discounted. We should be able to find this raw and processed data after you have graduated. Make sure that all your data files (both raw and processed) are attached to each notebook page.

Start each page with a date the experiment was started, a title, the purpose of the experiment (what you are doing & why), and your hypotheses. Add any references to the related literature and any previous notebook pages. Note that if you are repeating a procedure, you must record it as a new experiment. You can copy/paste from the previous experiment, but be sure to update it with any changes that you make, including quantities of starting materials used, workup conditions, chromatography conditions, etc.

Include a schematic for the experimental setup if it is the first time (or reference a previous one). For research materials, include the source, product #, lot #, quantity and purity. For equipment, include manufacturer, location, parameters used.

See below for specific instructions that depend on the type of experiment you are doing. At the end of each notebook page, have a discussion/conclusion section that summarizes what was learned and the next steps.

## Experiment Pages - for syntheses

For syntheses, add a reagent table that includes molecular weights, mols/equiv, masses or volumes. Record masses based on the accuracy of the balance, and volumes based on the accuracy of the syringes. Record the source of each reagent (lab notebook page or commercial supplier), the date opened and the batch number (if purchased).

Record the actual quantities added to the accuracy of the instrument you used to measure it. For example, if you intended to add 10 g and you weighed out 10.230 g - record the 10.230 g. Be sure to re-calculate the mols/equiv based on what you actually measured, not what you intended.

Make sure to include the time at which you start the experiment as well as when you finish it. If you work on the experiment over multiple days, record a new date and time for each part of the experiment on the same notebook page.

Record every action and observation. The more detail you provide, the easier it will be for you (or someone else) to learn from and reproduce your work. Use past tense to describe the experiments. Use full sentences, in paragraph form.

Be sure to indicate the time involved for all steps (e.g., stirred for 3 h) and the temperature (e.g., at rt). Always indicate whether the reaction was performed under inert atmosphere (e.g., under N<sub>2</sub> or in the glovebox) or ambient conditions (e.g., open to air).

If you are doing an action, like a freeze-pump-thaw cycle or bubbling H<sub>2</sub> through your solution, be sure to indicate the times (e.g., for 10 min) for each step.

Estimate approximate volumes for workup conditions (e.g., approx. 10 mL of water was added to quench the reaction), including LLE (e.g., ~50 mL of DCM was added and the organic layer was separated).

Provide explicit details about what you see: Is the reaction homogeneous or heterogeneous? Does that change over the course of the reaction? Is there a color observed? Is your product colored?

If you used a reagent that required some purification, be sure to state that here, ideally referencing another notebook page where that purification was recorded. Similarly, if you are

If you prepare a sample for analysis, state how that sample was prepared (e.g., 0.05 mL of the crude reaction mixture was diluted with 2 mL Et<sub>2</sub>O, then filtered through a small plug of silica and analyzed using the “lower-high” method on the GC-MS).

Indicate in your notebook the file name and date acquired for all data relating to that experiment. You should also include pertinent information about the instrument the data was acquired on.

Describe the data in your own words; what does this data mean with respect to this experiment and your future plans?

both column fractions looked exactly the same

EAM\_4-1-147\_F\_2B-  
Proton Spectrum

The NMR spectrum shows intensity in arbitrary units (0 to 350) on the y-axis and chemical shift in ppm (10.5 to -1.0) on the x-axis. The following table summarizes the observed peaks:

| Chemical Shift (ppm) | Approximate Intensity |
|----------------------|-----------------------|
| 7.84                 | 100                   |
| 7.63                 | 280                   |
| 4.05                 | 140                   |
| 2.45                 | 350                   |
| 1.602                | 60                    |
| 1.33                 | 140                   |

response factors

21

**Conclusion:**

First issue: added 10x the amt of catalyst I wanted to. Next time will be careful to add less! Next, the product co-elutes with C22 (DUH), so will need to change GC standards before running this experiment again. I'm guessing low conversion is because the catalyst died (turned black). Will try again but leave the reaction at 0 the whole time. JACS paper cited above seems to indicate that changing the eq of grignard won't have a large effect on yield (even tho I'm seeing some mono-funct).

## Experiment Pages - for microplastics research

### Sample identity and preparation

Indicate the amount of sample used by mass or volume.

*For generated solutions:* indicate the solvent, concentration, volume, and how the solution was mixed.

*For generated particles:* cite the notebook page for samples that were created in-lab along with any characterization data of the generated samples.

*For commercial standards:* detail the supplier, batch number, size, shape, identity, density, and color.

*For environmental samples:* indicate the origin and any previous isolation attempts (i.e., sample history).

### Experimental details

List the protocol for preparing all solutions including filtering conditions (type of filter), solvent, type of filtration, and components.

Include glassware cleaning conditions and substrate preparation protocol, if any.

Note experimental observations and time conditions of all reactions (e.g., digestion).

*For environmental sampling:* include information on location, date, weather conditions, description of instrumentation or tools used, time of collection, images of collection, and note plastic use.

*For microplastic capture:* include information on pump model and rate, details on flow conditions, capture medium, material for capture (pore size, mass, layers), tubing identity, and include an image of the setup.

*For microplastic extraction and isolation:* include information on chemical supplier information and concentration, digestion protocol, density separation protocol, staining protocol, and resting time (if applicable).

*For probe tack:* include information on method parameters, probe material, any sanding completed for polymer probes, the number of samples, probe pokes per sample, film thickness, sample preparation procedure, observed thickness via microscopy, and link the adhesive synthesis notebook page.

### Analysis information

Include the name of any assistants and their contribution to your results.

List the location, name, and parameters of any instrumentation used.

Include information on the number of samples or particles analyzed as well as a description of subsampling protocol, if any.

Export and link raw files or indicate the file location if they are too large to attach in OneNote.

Include searched libraries, software, and conditions of spectral identification.

*For SEM:* include information on citation/acknowledgement criteria, sputtering time and coating type, detector used, high voltage, beam intensity, magnification, and view field.

*For optical image collection:* include information on the magnification, number of tiles in mosaic, and indicate whether a mosaic or single image was collected.

*For flow cytometry:* include information on acquisition volume, flow rate, stop option and value, and voltage setup.

## Experiment Pages - for e-chem/battery research

### Stock solutions

Oftentimes we use stock solutions (e.g., 0.5 M KPF<sub>6</sub> in MeCN) so it is helpful to either make a notebook page which details how you make your stock solutions or include those details in each experiment.

Important details to include are: solvent supplier and grade, electrolyte supplier, if electrolyte was recrystallized, how it was recrystallized (solvent(s) volume, solid volume, temperature, time), how electrolyte was dried (vacuum oven, temperature, time).

Were the stock solutions dried over sieves in the glovebox (size, brand, pretreatment)?

### Electrodes

How were the electrodes made? What materials were used? Where were they purchased? How are they cleaned or polished? What solution is contained in your reference electrode? When was the reference electrode prepared / how long has it been used?

### Material synthesis

Hyperlink synthesis notebook page and include how the material was dried before bringing it into the glovebox.

### Procedure notes

How was the experiment set up? What electrodes were used? Solvents? What settings were used on the potentiostat?

CV: reference electrode, counter electrode, working electrode; vessel (e.g., 20 mL vial); concentration of material and supporting electrolyte, scan rate

BE: galvanostatic? CCCV? Electrodes?, capacity cut off, voltage cutoff, charging rate, number of cycles

Electrasyn: anode, cathode, volume, current/voltage, time, reference electrode (if used), stirring rate, alternating current (if used)

Battery: Electrodes (any pretreatment?), gaskets, O-rings, membrane/separator, flow field, volume, concentration, flow rate, tubing (on the cell and the pump), EIS conditions, GCPL conditions (or other technique)

### Characterization data

Include all raw data on an excel sheet and make sure the file name corresponds to the notebook page. If data needs to be further worked up, include those excel sheets too.

Include a few sentences to explain results (what were you looking for and what did the experiment tell you?)

It is also helpful to include all raw data files in your notebook. This can be done by saving the folder containing the raw data as a .zip file and uploading it to the notebook page.

### Summary

Ultimately, your electronic lab notebook, collections of spectra and other data, and the supporting information documents are the ***most important*** things you will prepare as a scientist during your PhD. You should take pride in these items and spend the time to prepare a solid foundation to support your claims. This documentation can and will be used to verify that indeed these experiments were run and that the results are as you claim. If there are errors in these records, then it can call into question deeper issues ranging from carelessness, negligence, to scientific fraud. These can result in serious consequences, including getting expelled from the PhD program. **Do not take these issues lightly!**

## A note about significant figures, means, and standard deviations

Please see the errors presentation on the McNeil Group shared Google Drive for the full explanation; copied here is the brief summary.

### Significant figures

Significant figures include all the digits you are certain about PLUS one additional uncertain digit. Note that our balances are uncertain in the *last* digit you can read (e.g.,  $\pm 0.1$  mg).

### Counting significant figures

Leading zeros are not significant. 0.008 has one significant figure

Captive and trailing zeros are significant. 1.02 has three, 40.00 has four significant figures

### Some instruments report a dozen or more numbers for a data point, how many values should I include in subsequent calculations?

Carry one extra digit (beyond the last significant figure) through to the final result and then round. You may need to do some digging online or in the instrument manual to understand the precision of each instrument.

### Rules for rounding

Round up or down based on the number adjacent to the last significant figure. (4.348 becomes 4.3) If the digit is 5, then round to the closest even number. (1.35 = 1.4 and 1.65 = 1.6)

### Random errors

Cause replicates to fall on either side of the mean; can be minimized with better techniques

### Mean

The (arithmetic) mean is the sum of all the values divided by the number of observations. Use the “average” function in excel or sheets.

### Standard deviation

Quantifies the deviation or spread in a series of data relative to the average. Use the “stdev.s” function in excel or sheets.

### Significant figures with standard deviation

Your error should only contain one significant figure (e.g.,  $\pm 1$  or  $\pm 0.5$ ) and your average should then be reported to this same level of precision (e.g.,  $4 \pm 1$  or  $4.1 \pm 0.5$ ).

### Relative standard deviation (needed for calculations)

Unitless (percent) deviation that can be used to compare precision across experiments and calculate error (sig figs) in equations where different measurements (e.g., mass and volume) are combined. It is the  $\text{std dev}/\text{mean} * 100$  or for a single measurement  $\text{std dev}/\text{value} * 100$ .

### **Propagating errors**

Linear (addition/subtraction) is the square root of the sum of the individual squared std dev.  
Multiplicative (multiply/divide) is the square root of the sum of the squared rsd.

### **Reporting calculated values**

Once you have propagated the error in each of your individual calculations and determined the rsd for the final calculation, multiply this rsd by your calculated value to determine the number of significant figures to report. For example, if your rsd is 0.9% and your calculated value is 13.432, you would report it as  $13.4 \pm 0.1$ .

## Labeling and storing materials

Label all vials with a structure AND the notebook page number. Use a small white label and attach to the vial with reinforced clear tape. Sharpies do not last the test of time! Indicate the amount of material inside the vial on the screwcap (e.g., 52 mg).

Store all synthesized materials in small disposable vials with screwcaps. Please do not store any compound in an expensive flask with ground glass joints. Store all synthesized compounds either near your bench or in your assigned shared refrigerator. Do not store your compounds on the group chemical cabinets.

## Mentoring checklist

*Please complete the following checklist with your mentor, and return a signed, scanned copy as a pdf file to Anne and upload a copy to the McNeil Group "Shared Drive" mentoring folder.*

| <i>Trained</i>                  | <i>Proficient</i> | <i>Task / Skill</i>                                                                                                                                                    |
|---------------------------------|-------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Safety</b>                   |                   |                                                                                                                                                                        |
|                                 |                   | I have completed the "lab entry - safety checklist" and sent a PDF copy to Anne and uploaded it onto Drive.                                                            |
|                                 |                   | I understand how to be a safe worker in the lab on my specific research project and have demonstrated it.                                                              |
|                                 |                   | I understand what "good chemical hygiene" refers to (clean workspaces, clean shared spaces, returning chemicals to their original location, etc.) and demonstrated it. |
| <b>Navigating the lab</b>       |                   |                                                                                                                                                                        |
|                                 |                   | I understand what is expected of me from subgroup presentations.                                                                                                       |
|                                 |                   | I understand what is expected of me for the online laboratory notebook pages and how to store/backup my data.                                                          |
|                                 |                   | I am properly storing and labeling my samples.                                                                                                                         |
|                                 |                   | I can navigate to shared online resources like training manuals, Drive, and library/web resources.                                                                     |
|                                 |                   | I know how to search the department's chemical inventory and how to order supplies and reagents.                                                                       |
|                                 |                   | I understand the group guidelines on how to make figures.                                                                                                              |
|                                 |                   | I have watched tutorials for ChemDraw and Adobe Illustrator and can use those for my presentations.                                                                    |
| <b>Searching the literature</b> |                   |                                                                                                                                                                        |
|                                 |                   | I have demonstrated effective searching using Reaxys, SciFinder, and Web of Science.                                                                                   |
|                                 |                   | I have set up alerts for research papers related to my project.                                                                                                        |
|                                 |                   | I have crafted a preferred method to save and annotate papers related to my project (e.g., Zotero, Notability, etc).                                                   |

|                                                                |  |                                                                                                      |
|----------------------------------------------------------------|--|------------------------------------------------------------------------------------------------------|
|                                                                |  | I have used some online library resources like e-EROS.                                               |
|                                                                |  | I have used an online chemistry resource including Not Voodoo, SafetyNet, etc.                       |
| Reading a paper effectively                                    |  |                                                                                                      |
|                                                                |  | I have demonstrated that I can read a paper effectively and write short summaries of the key points. |
|                                                                |  | I understand how to read papers for specific information versus general background.                  |
|                                                                |  | I am an active participant at the professional development meetings.                                 |
|                                                                |  | I read papers before the seminar by the speaker.                                                     |
| Basic synthetic lab techniques (if applicable to your project) |  |                                                                                                      |
|                                                                |  | I can safely operate the Schlenk line and vacuum pumps (and gauges).                                 |
|                                                                |  | I can safely syringe and pipette solutions.                                                          |
|                                                                |  | I can safely dispose of solid, liquid, and sharps waste.                                             |
|                                                                |  | I have demonstrated that I can run and analyze TLC plates.                                           |
|                                                                |  | I have demonstrated that I can successfully run a column by hand.                                    |
|                                                                |  | I have demonstrated proper use of a rotovap and can disassemble it for cleaning or repair.           |
|                                                                |  | I have demonstrated proper cleaning and drying of glassware.                                         |
|                                                                |  | I can take an $^1\text{H}$ NMR on my own (not on "Carbon") and interpret it.                         |
| Project-specific training                                      |  |                                                                                                      |
|                                                                |  |                                                                                                      |
|                                                                |  |                                                                                                      |
|                                                                |  |                                                                                                      |
|                                                                |  |                                                                                                      |
|                                                                |  |                                                                                                      |
|                                                                |  |                                                                                                      |

# Expectations for publishing

## The paper-writing process

### Stage 1

Before drafting any manuscript, you should compose an outline. I recommend going through all your old subgroup files to remind yourself of all the experiments you did. Schedule a meeting with Anne to outline the tentative paper. Come prepared with an outline.

### Stage 2

Download the appropriate journal template and begin writing. You have (at most) four rounds of revisions, where Anne provides hand-written comments on your writing. Use your judgement, then, about when the first draft is polished enough to send along. (I recommend having a senior/experienced student read your first draft and provide comments before sending it to Anne.) After four rounds of revision, Anne will “take over” and finish it up. The goal is for you to improve your writing each time so that your next manuscript’s first draft starts at the level where you left off. During this time, you should also be compiling the necessary supporting information file. Please see the guidelines in this manual and use the SI template. Again, use your peers for feedback before sending the first drafts to Anne. \*\*Please DO NOT use any reference manager to insert your references. Instead, use MS Word “insert” “endnote” or “insert” “cross-reference.”

### Stage 3

At this point, Anne is polishing the text and figures, and may request additional figures or data (i.e., experiments). The most useful thing you as an author can do at this point is help with identifying appropriate references by performing comprehensive searches. In addition, it is at this point that the SI file should be edited and approved by Anne and then sent out for group edit. You are responsible for incorporating the group edit changes to the SI.

### Stage 4

The manuscript will go through a group edit, usually with Anne incorporating the final changes and getting ready for submission. The SI file should be finalized and ready for submission. Anne will draft the cover letter and ask you for suggested reviewers.

### Stage 5

Most papers these days go through at least 1 round of revision. For your first paper, Anne will handle the revisions while sharing the information and process with you. If this is not your first paper, you will have a chance to draft the response to reviewers and revision cover letter.

## How to write a good paper

The following information was drawn from group exercises that took place in May 2019, Fall 2021, and Fall 2024. Each time, we looked at ~20 papers and individually voted on whether we liked each title, abstract, intro, results/discussion, conclusions, figures, and commented on what we liked or didn't like about them. Then we came to a consensus on what makes a good one "good", and what to avoid.

### Titles

#### Good titles...

- we can understand exactly what was done
- contains the "what" and the "how" (in that order) or contains take-home message
- are between 6-15 words
- contain action words (e.g., predicting, tuning, etc.)
- start with the keywords most relevant to the work
- are not too generic to preclude future publications

#### Bad titles...

- contain unnecessary words (e.g., synthesis, properties, design, toward, use in, etc.)
- contain redundant words
- start with "a"
- have unnecessary adverbs and/or excessive prepositions
- use colons
- contain complex words
- are too long (>15 words)
- are too short (<6 words)
- hard to tell what is new or interesting
- have too little information
- missing the "how"
- use unfamiliar acronyms or abbreviations
- oversell the article
- force fit catchy terms (e.g., "keep xx on track," "strike a balance")

#### Examples of good titles...

- Influence of Counterion Structure on Conductivity of Polymerized Ionic Liquids

## Abstracts/TOC graphics

### Good abstracts...

- contain five sentences/sections in this order:
  - (1) challenge/problem statement - what are you trying to solve/address/understand
  - (2) how did you go about addressing it (not too detailed)
  - (3) what did you actually do (more detailed)
  - (4) what are the most important results (should relate to your challenge/problem statement); minimize quantitative data
  - (5) impact/importance of the results
- are self-contained
- use clear, simple language that is understandable to the journal audience

### Bad abstracts...

- are missing any one of the 5 sections mentioned above
- contain too much raw experimental data
- contain a lot of technical jargon and acronyms/abbreviations (think about your audience)
- use strong words that are a matter of opinion (excellent, versatile, synergy)
- contain too much of one thing (e.g., results)
- unclear on the key take-home message of the work

### Good TOC graphics...

- present a single take-home message in cartoon format

### Bad TOC graphics...

- overly complex with multiple take-home messages
- use actual data plots that require one to take the time to interpret
- contain neon green or other offensive colors
- are too technical (e.g., photos of polymers before/after stretching with ruler)

### Example of a good abstract & TOC graphic (here and here).

## Introductions

### Good introductions...

address these questions

- what is the problem/challenge that you are trying to solve?
- why does it matter? why do we need to solve it? why is it interesting?
- what is your approach/hypothesis about tackling this problem? what is the rationale?
- what are your most significant findings? provide context to understand them
- how do your findings impact the field?

general guidelines

- open with the need and then follow with your approach
- similar to a funnel, start broad and gradually narrow
- consider using shorter, digestible paragraphs
- each paragraph should have a smooth transition from the previous one
- clearly explain all key concepts that are necessary to understand the work/context without getting into the nitty gritty details
- contain 0-1 simplified scheme

### Bad introductions...

- are too long (we found ~600-1000 words was appropriate for full papers)
- are disorganized, jumping around from concept to concept without a clear understanding of where it's going
- no clear gap or challenge stated
- too repetitive
- have too many gap statements and its not clear which one(s) are being addressed
- not clear why the work is needed or what was learned
- no hypothesis stated or rationale for why they thought their approach would work
- includes equations and undefined complex concepts that are specific to a subfield
- include specific results (e.g., #) without context to understand them

[Example of a good introduction \(full papers\)...](#) [\(link and link\)](#)

[Example of a good introduction \(communication\)...](#) [\(link\)](#)

## Results & discussions

### Good results & discussions...

- Tell a story from start to finish, bringing the reader through the project with multiple guideposts that recap what was learned and inform on what is coming next.
- Consistent paragraph structures:
  - Rationale for why the upcoming experiments were done (1-3 sentences).
  - Description of key results (3-5 sentences).
  - Rationalization of the results (1-3 sentences)
  - Implications of the results. What does this mean for the story and/or the field? (1-3 sentences)
- Each paragraph should have a single goal or take-home message.
- Abbreviations with meaning - for example NBE for norbornene as opposed to M1.
- Use descriptive text that will be understandable to a non-expert.
- Figures should tell the story without text. Use of color, cartoons, and schemes to help guide data interpretation were all highly valued. See [here](#) for a really good example.
- Transitional phrases were really helpful. “We hypothesized” “We anticipated” “To understand” “When then rationalized that”
- Used sub-section headings to help guide the reader on how the parts connect together.

### Bad results & discussions...

- Make the reader work hard to understand the results.
- Have disparate sections that seem unrelated without transitional phrases or sub-section headings between them.
- Descriptions of results without a clear understanding of why the experiments were done.
- Descriptions of results without their implications.
- Contain too many abbreviations and acronyms. It breaks up the flow of sentences and makes the reader work harder to understand/comprehend the experiments.
- Contains too much numerical data rather than describing trends in the data or the implications of the data.
- Talk extensively about figures located in the SI.

### Example of a good results & discussion... (link and link)

## Figures/charts/schemes

### Good figures/charts/schemes...

- The reader looking at the figure/chart/scheme can immediately understand what the “take-away” message is without having to read the caption or main text.
- Have one key take-away message per figure/chart/scheme. Do not try to convey too much information in one.
- Use complementary colors (and not too many of them) to highlight important features or structural changes. Shading in parts of structures can also be useful rather than using bold or a lot of colors.
- Use consistent capitalization, fonts, and font sizes throughout.
- Use consistent structure sizes and specs throughout.
- Are symmetrical and minimize white space.
- Often include a cartoon depiction of the experiment alongside the data for easier interpretation.
- For complex or large structures, include both cartoon and chemdraw versions in the same figure and use the same cartoon throughout the paper.
- For multiple spectra, consider using dotted lines to label peaks from one to another rather than individually labeling or coloring peaks.

### Bad figures/charts/schemes...

- The reader must also read the caption and main text to understand the “take-aways” from the figure/chart/scheme.
- Are too busy with too much information trying to be conveyed.
- Contain too much text or a lot of duplicated text.
- Contain a lot of different data types without a clear understanding of what is being done in each experiment, and how they relate to each other (if at all).
- Make the reader work too hard.
- Use things like i, ii, iii and then never define them in the figure or caption.

### Examples of good figures/charts/schemes... (link and link)

## Conclusions

### Good conclusions...

- have these basic sections
  - a brief statement about why the work is important/necessary/significant
  - a brief summary of their approach (1-2 sentences)
  - a brief summary of the key results and context for those results (how does this compare to other materials/work in the field?)
  - an explicit discussion of the implications of the work (1-3 sentences) including potential limitations and how that would inform future work of the field
- shorter sentences with simple words/terms were best
- 1-2 paragraphs preferred
- define all terms (even if defined in the paper b/c some people read the conclusion after the abstract)
- ok and maybe even helpful to include cross-references, and/or new references to support the impact statements

### Bad conclusions...

- re-hash their discussion of the key results (e.g., “using MALDI to determine end-groups, we...”)
- contain too many value judgement or useless words (e.g., versatile, excellent, envisaged, first, etc)
- contain too much numerical data/results
- rely on acronyms introduced in the paper but not in the conclusions
- reference figures or SI
- Includes too many takeaways or the take home message is not clear

## ChemDraw guidelines

Open the [McNeil Group Chemdraw Template](#). There are a lot of great tutorials [here](#) and [here](#) on the web for learning and mastering ChemDraw. There is also a comprehensive 300+ page [user guide](#) and list of [shortcuts](#).

- Pay attention to the little details, like centering text over arrows, aligning and distributing the structures in a reaction, using the same sized arrows in a single scheme and paper.
- Color can be a really useful tool. Pick one of the two color schemes in our template and stick with the same one throughout your paper/talk.
- Never leave a bond “empty”, if it is a methyl group then add the label, but do not switch between CH<sub>3</sub> and Me within a paper or talk. Pick one.

When you are ready to “move” your structures into another document, save your file as both a .cdx and (save as) .png. You can copy/paste your structures directly into your presentation. For papers, on the other hand, some more work is required.

- Open the png file in Photoshop. Then go to **Image** and choose **Image Size**. Use a calculator to determine the new width and height (in inches or cm) by multiplying the original values by some %. The smallest size you should re-size a ChemDraw image is 65%. If that is too small for your preferences, try 70%. Most importantly, once you pick a re-size value, stick with it for all images within a single paper. Note that for single column figures, the max size is 3.3 in and for double-column figures, the max size is 6.5 in.
- In some cases, you may want to add your ChemDraw scheme into a larger figure in Adobe Illustrator. You can either open and modify the original png file (before resizing) and then resize your entire image at the end by 65% or 70% before inserting into Word. Or you can work with your resized Chemdraw file and make sure your Illustrator image does not exceed the margins required for use in Word without resizing.

# Plot/figure/scheme/chart/table guidelines

## Plots

All plots should be created in Prism or SigmaPlot. The plot size should be square; I recommend setting the plot dimensions to 3.0 x 3.0 inches. Almost all plot axes should start at 0,0 unless it really doesn't make sense to do so. The axis labels should be simple, and contain the units in parentheses. Also, do not capitalize the axis labels. The data on the plot should be clear/readable and labeled so that the take-home message is easily interpreted. Please do not use "legends" or figure captions. The plot itself should be self-explanatory. Use color sparingly; use grayscale and dashed lines as a starting point.

Please follow the follow guidelines for plot formatting:

Plot dimensions: 3.0 x 3.0

Axis and Tick Sizes: 3 pt (only use major ticks)

Axis Font: 16 Arial Bold

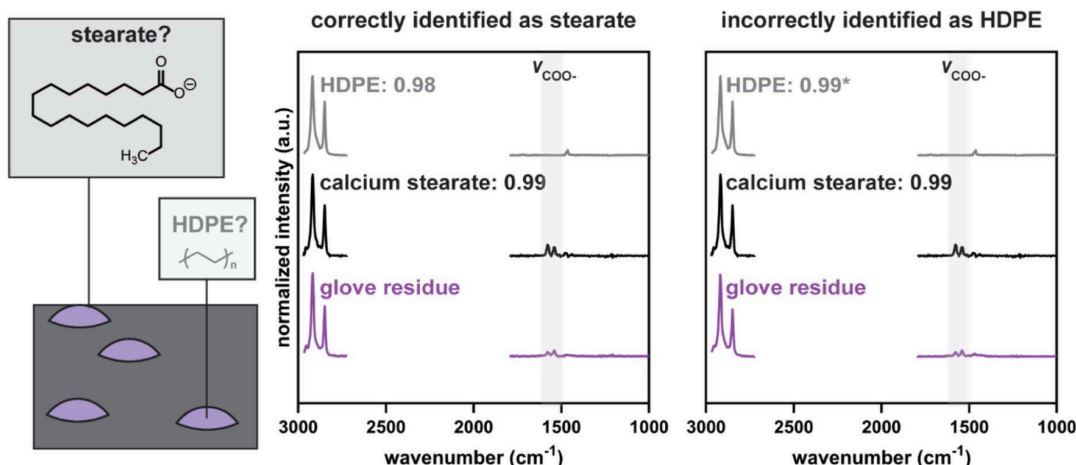


Fig. 5 PTIR spectra of stearate glove residue alongside reference spectral matches with topmost hit quality index (HQI) for spectra identified as calcium stearate and high-density polyethylene (HDPE) by traditional library matching methods. The distinguishing carboxylate stretch region of the spectrum is highlighted, and the asterisk indicates a higher HQI by less than 0.01.

## Figures

First and foremost, figures have processed data (plots, spectra, etc). Sometimes chemical structures and/or reactions can be added to supplement the data, but a figure must have some data! In general, stick to one column figures (width 3.3 cm) unless there is a really strong justification for using the two column width (6.5 cm). Note that two plots can fit side-by-side into a single column figure without appearing too small. Figure captions should be concise and contain essential experimental information!

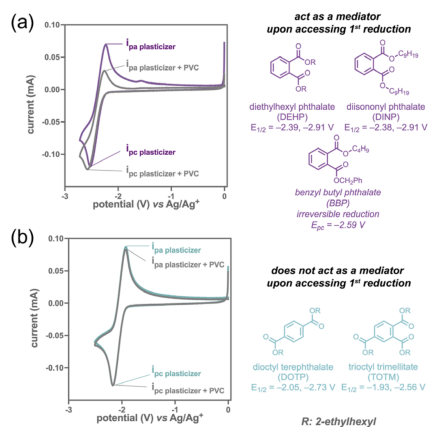
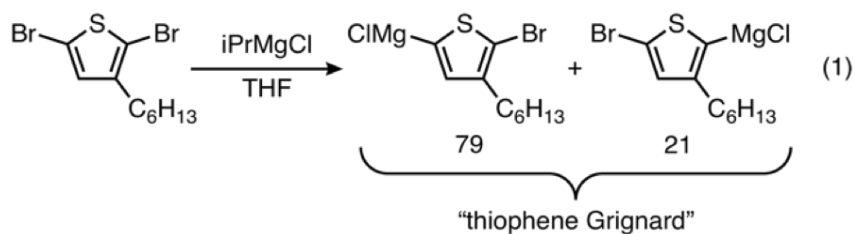


**FIGURE 1** | (a) Plasticizers that act as a mediator in their first reduction with a representative cyclic voltammogram of DEHP with and without PVC at a scan rate of 100 mV/s. (b) Plasticizers with no mediator behavior in their first reduction with a representative cyclic voltammogram of DOTP with and without PVC at a scan rate of 100 mV/s. Reduction potentials ( $E_{1/2}$ ) are referenced to  $\text{Ag}/\text{Ag}^+$ . Due to BBP's irreversibility, the reduction at the peak cathodic current ( $E_{pc}$ ) is reported. Concentrations include  $\text{PVC}_{37k}$  (30 mM), plasticizers (10 mM), and  $\text{NBu}_4\text{BF}_4$  (0.1 M) in DMF, whereas  $i_{pa}$  and  $i_{pc}$  refer to the anodic and cathodic peak currents, respectively.

## Equations

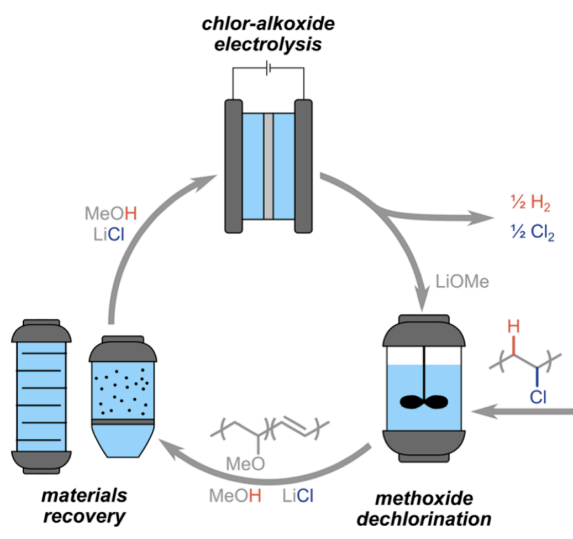
Equations usually contain either mathematical relationships or a single chemical transformation. Number them sequentially in the manuscript (hint: place the # in the chemdraw version to keep the sizing the same). Equations do not contain titles or captions.



## Schemes

A scheme is a series of equations that make more sense when grouped together. A good rule of thumb is that if it has more than one reaction arrow, it is likely better represented as a scheme. Schemes require titles which are generally placed above the chem draw (though be sure to check the journal requirements). The title should briefly describe the main conclusions of the scheme.

**Scheme 1. Envisioned Electrochemical Chlor-alkoxide Process to Generate Chlorine and Hydrogen from Waste PVC**



## Charts

A chart is a collection of structures, sometimes with data associated with them. Chart titles are generally placed above the data (journal specific) and briefly describe the major findings.

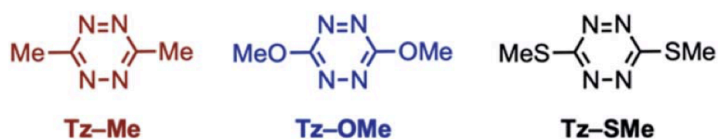


**Chart 1** Tetrazine scaffolds explored in this work.

## Tables

I generally avoid tables unless absolutely necessary. Sometimes reviewers insist on them! Tables are most useful when you run a series of reactions with varying conditions or substrates. Before making a table, consider whether a chart might be a better method of presenting the data.

**Table 2. Dry Thickness, Ionic Conductivity, and Voltage Efficiency Values for AEMs in MeCN and PC**

| AEM         | dry thickness ( $\mu\text{m}$ ) | ionic conductivity ( $\mu\text{S}/\text{cm}$ ) |                 | voltage efficiency (%) |            |
|-------------|---------------------------------|------------------------------------------------|-----------------|------------------------|------------|
|             |                                 | MeCN                                           | PC              | MeCN                   | PC         |
| FAP-330     | 32                              | $317 \pm 7$                                    | $168 \pm 4$     | $87 \pm 1$             | $80 \pm 1$ |
| FAPQ-330    | 36                              | $390 \pm 10$                                   | $151 \pm 3$     | $90 \pm 1$             | $74 \pm 1$ |
| FAP-450     | 56                              | $560 \pm 10$                                   | $231 \pm 4$     | $95 \pm 1$             | $78 \pm 1$ |
| FAPQ-375-PP | 107                             | $440 \pm 10$                                   | $78 \pm 3$      | $90 \pm 1$             | $34 \pm 1$ |
| FAP-330-PE  | 45                              | $263 \pm 8$                                    | $81 \pm 1$      | $95 \pm 1$             | $66 \pm 1$ |
| FAM         | 526                             | $19.7 \pm 0.03$                                | $0.88 \pm 0.03$ | $21.0 \pm 0.5$         | n.d        |
| AMI-7001S   | 568                             | $110 \pm 3$                                    | $1.17 \pm 0.05$ | $33.5 \pm 0.5$         | n.d        |

## Supporting information guidelines

### philosophy

This document is incredibly important and one that should replicate the results you obtained as depicted exactly in your lab notebook. Every section of SI should be associated with an experiment number from your notebook and data files. Before we submit a paper, you must submit to Anne (and post in your folder on the group Drive) a copy of the SI with each notebook page indicated for each experiment. Original electronic copies of the raw data must also now be submitted as a single XLS file (see new publication data guidelines). Your notebook details, raw data, and SI must match exactly or you will be asked to re-run the experiment again prior to submission.

Note: We have a SI group template; follow those instructions/guidelines.

For the table of contents: You should list both the section titles as well as their starting page #. The section titles should be informative but not too lengthy, and written in sentence case. The order of sections should follow the order in which the data appears in the paper.

### common general formatting mistakes/reminders

- Margins need to be justified.
- A regular hyphen (-) is used to separate elements of a compound word (i.e. “water-soluble”).
- The en-dash (-) ([option][-] on a Mac) is used for things like named reactions (“Diels-Alder”), number ranges (“1-13”), bonds (“C-O bond formation”), or negative temperatures (i.e.  $-35\text{ }^{\circ}\text{C}$ , not  $-35\text{ }^{\circ}\text{C}$ )
- Degree signs ( $^{\circ}$ ) should be written using [option 8 on a Mac] not using a superscript o.
- There should be a space between the numbers of a temperature and the degree sign (i.e. “ $55\text{ }^{\circ}\text{C}$ ”, not “ $55^{\circ}\text{C}$ ”).
- Abbreviations: h not hours; min not minutes; d not days; s not seconds.
- Check all elemental formulas and mass spec formulas for errors/typos.
- Using fewer words is preferred (e.g. “synthesizing” not “the synthesis of”).
- Use proper and consistent nomenclature for compounds.

- HRMS  $[M + H]$  versus  $[M + H^+]$ . Make sure that your molecular formula corresponds to the peak that you're reporting. For example, if a proton ( $H^+$ ), sodium cation ( $Na^+$ ), etc. is present in your peak, it should also be in your molecular formula.
- Compounds, schemes, and tables should be numbered sequentially. Compounds that do not appear in the MS should be given an S number (e.g., Compound S1).
- Amounts of reagents, solvents, etc. are set aside parenthetically. For example, "The solution was washed with brine (3 x 50 mL)," not "The solution was washed three times with 50 mL of brine."
- "That" and "which" are not interchangeable! If removing the words that follow would change the meaning of the sentence, use "that". Otherwise, "which" is fine.
- "Et al." and "and coworkers" are not interchangeable. Smith, Leone, and McNeil\* would be "Smith et al." or "McNeil and coworkers." I prefer the "and coworkers" approach for easier attribution and retrieval of the literature.

## syntheses

### Materials and supplies

Should list the source of reagents and materials, whether and how they were purified before use, and batch or lot number.

### General experimental

Should give specific information about the types of equipment used, and if appropriate, how the samples were prepared and analyzed.

### Synthetic procedures

Should describe how materials generated during the course of the work were made. It should be self-contained, meaning that if you had to make it for this paper because it was not commercially available, then its synthesis should appear here...even if we (or someone else) previously published a synthetic procedure for it. Undoubtedly, you did it a little differently, and the SI should represent your individual work and should match the referenced notebook page exactly! In addition, you should list either the elemental analysis results OR high res mass spec results which support the identity of the compound.

### Characterization

Should include all "characterization" (e.g.,  $^1H$ ,  $^{13}C$ ,  $^{19}F$  NMR spectra) of the compounds made in the synthesis section. The figures should all have the same x-axis scaling (e.g., 0-8 ppm for all  $^1H$  NMR spectra). Be sure to check the journal if any particular guidelines are required for submission. I recommend making a template of just the axes and then pasting the spectra (without axes) into the template for consistency. Each figure should also have chemical structure and structure number. If the peak splitting is hard to see, then insets should be created as well. The figure caption should list the peak positions to 2 decimals (both  $^1H$  and  $^{13}C$ ), coupling constants (italicize the J), and the number of protons (based on the integration).

## microplastics

### Materials and supplies

Should include supplier information for any materials acquired (part number, lot number, size). Include suppliers of any substrates or small instruments (e.g., pumps used for active sampling). For commercial microplastics, include the size, shape, supplier, batch number, density.

### Quality assurance/quality control

Should describe all procedures used to limit contamination, including your cleaning protocol, types of glove used (if applicable), type of hood used (e.g., laminar flow). Note which steps use plastic materials. Describe positive controls and procedural blanks, and include mass recordings, microscopy images, and spectroscopic data.

### Experimental section

Describe the sample collection process. Include photos of the experimental setup. Describe the extraction protocols used (depending on type of experiment-digestion, density separation, filtration, concentration and volume of reagents, staining and resting time). Include any relevant details related to the conditions at the time of sampling, including pumps used during active sampling (pump rate, flow conditions, capture medium, materials for capture, tubing identity).

### Study area/sampling location

Provide the address and coordinates, include a map if available. Indicate when samples were collected (month, season), weather patterns, and methodology (How were samples collected? What equipment was used?) Include specific details depending on the project (i.e., height/angle at which sampler is placed, depth at which water or soil samples are collected, quantity of water or soil collected). Pictures are helpful here too!

### Data

For all data analyses, include instrument settings (i.e., laser power, preprocessing, number of scans, relaxation time, objective, wavelengths, spectral resolution, flow rate, limit of detection, analysis protocol- library search/manual/conformal prediction). Include all filter images: optical, fluorescent, etc. Include all spectra: IR, Raman, O-PTIR. Include any additional characterization: DSC, TGA, etc. Include individual microplastic images from the instrument used to collect spectroscopic data

For all spectral analyses, provide details on how analysis was performed. Include the number and size range of particles analyzed. Provide information on the percentage area of substrate that was analyzed (was the whole substrate analyzed or sub analyzed? If the latter, how were areas/particles chosen?) Label all characteristic peaks

### Statistical Data Processing

Explain all steps taken during data processing (e.g., pre-processing, baseline optimization, normalization, etc). If using a model to label spectra, provide full background information on how it works.

## electrochemistry

### Materials

Describe the purity, lot number, and manufacturer for all reagents used. Describe any recrystallization, purification, and drying procedures

#### I. Materials

Dichloromethane (DCM) was dried and deoxygenated using an MBraun solvent purification system composed of activated alumina, copper catalyst, and molecular sieves. All other reagent-grade materials and solvents were purchased from Millipore Sigma, Fisher, Oakwood, or Alfa Aesar and used without further purification.

3,6-Dimethylthio-1,2,4,5-tetrazine (Tz-SMe  $\geq 95\%$ , Lot: MKBx4007V) and silver hexafluorophosphate ( $\text{AgPF}_6$ , 99.99%, Lot: MXCS1412) were purchased from Millipore Sigma. 3,6-Dichloro-1,2,4,5-tetrazine (95%, Lot: A147845-015) was purchased from Ambeed. 10-methylphenothiazine (MPT,  $\geq 98\%$ , Lot: BXX8M-XL), 10-[2-(2-methoxyethoxy)ethyl]-10H-phenothiazine (MEEPT,  $\geq 98\%$ , Lot: LMT2C-WG), methyl viologen dichloride hydrate ( $\geq 98\%$ , Lot: A0467142), ferrocene (Fc, 99%, Lot: M08E012), N-bromosuccinimide (99%, Lot: A0347531), sodium thiosulfate ( $\text{Na}_2\text{S}_2\text{O}_3$ ,  $\geq 99.5$ , Lot: 187475), and ammonium hexafluorophosphate ( $\text{NH}_4\text{PF}_6$ , 99%, Lot: A0441062) were purchased from Fisher. Iron(III) acetylacetonate ( $\text{Fe}(\text{acac})_3$ , 99%, Lot:

### General experimental

Provide detailed information about instruments used, including the manufacturer, and relevant parameters used for measurements.

#### II. General experimental

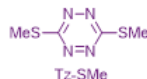
*NMR Spectroscopy* –  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra for all compounds were acquired at room temperature on a Varian VNMRS 600, Varian VNMRS 500, or a Bruker Avance Neo 500. Chemical shift data are reported in units of  $\delta$  (ppm) relative to tetramethylsilane (TMS) and referenced against deuterated chloroform ( $\text{CDCl}_3$ ), deuterated dimethyl sulfoxide ( $(\text{CD}_3)_2\text{SO}$ ) or deuterated acetonitrile ( $\text{CD}_3\text{CN}$ ).

*High Resolution Mass Spectrometry (HRMS)* – Data was obtained on a Micromass AutoSpec Ultima Magnetic Sector mass spectrometer using electron impact ionization (EI).

*Electrochemistry* – All electrochemistry experiments were performed with a VSP Bio-Logic potentiostat with capabilities for impedance spectroscopy from 10  $\mu\text{Hz}$  to 1 MHz, compliance voltage 20 V and current ranging from 10  $\mu\text{A}$  to 1 A. All experiments were carried out in an  $\text{N}_2$ -filled glovebox (MBraun Labmaster 130) with  $<0.5$  ppm water and  $<10$  ppm oxygen.

### Synthetic procedures

See above notes for “syntheses.” For all commercially purchased substrates, you need to verify both purity (e.g., using  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra) and identity (mass spec/elemental). For polymers, fully characterize them at the start as well (e.g., NMR spectra, elemental, TGA, SEC).



3,6-dimethylthio-1,2,4,5-tetrazine (Tz-SMe). Commercially available.

NMR:  $^1\text{H}$  NMR (500 MHz,  $\text{CD}_3\text{CN}$ )  $\delta$  2.70 (s, 6H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CD}_3\text{CN}$ )  $\delta$  172.80, 12.75 (Figure S1 on page S10).

HRMS (EI): Calc'd. for  $\text{C}_4\text{H}_6\text{N}_4\text{S}_2$   $[\text{M}+\text{H}]^+$  175.0107; found: 175.0112.

## Electrochemical methods

List all relevant information (current, potential, time, stirring, electrodes/where they were purchased, concentration of electrolyte solutions) so that anyone else can reproduce your experiment exactly as you did it. Include pictures and/or schematics of setups (if you want to include screenshots of the actual BioLogic parameters, do that too). If you're using a custom setup, include instructions and pictures of how to do that.

## Data

Recall that the order of the SI should correspond to the order of experiments in the paper. For calculations, initial raw data should be present, calculations do not need to carry raw data through every step but should show all steps and final results. If appropriate, include a page which summarizes the overall findings at the start of each data section. Put photos of samples after centrifuging, if relevant. Put photos of the cell before and after cycling, if relevant. Add descriptions of each variable in the equations (e.g.,  $F$  is Faraday's constant).

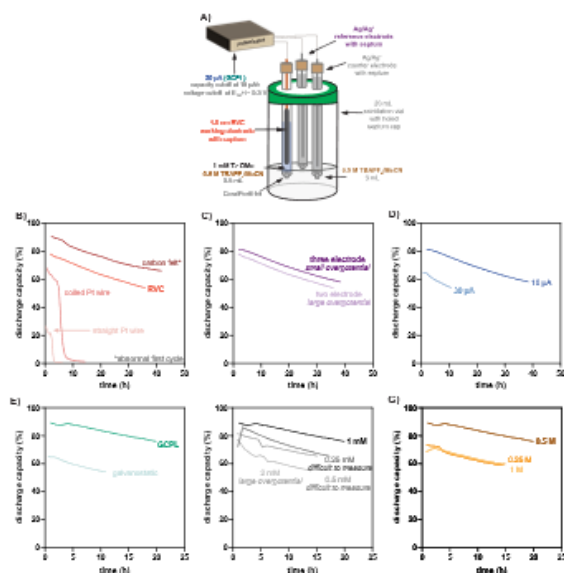


**Figure S14.** Summary of optimization cycling data, **optimized parameters in bold** (A) Schematic of optimized m-BE experimental setup. (B) Plot of discharge capacity versus time m-BE cycling of 1 mM Tz-OMe in 0.5 M TBAPF<sub>6</sub>/MeCN with a carbon felt (●), RVC (●), coiled Pt wire (●), and straight Pt wire (●) working electrode. (C) Plot of discharge capacity versus time m-BE cycling of 1 mM Tz-OMe in 0.5 M TBAPF<sub>6</sub>/MeCN in a **three electrode** (●) and two electrode (●) system. (D) Plot of discharge capacity versus time m-BE cycling of 1 mM Tz-OMe in 0.5 M TBAPF<sub>6</sub>/MeCN using a **30 μA** (●) and **10 μA** (●) galvanostatic charging rate. (E) Plot of discharge capacity versus time m-BE cycling of 1 mM Tz-OMe in 0.5 M TBAPF<sub>6</sub>/MeCN using a **GCPL** (●) and galvanostatic (●) charging rate. (F) Plot of discharge capacity versus time m-BE cycling of **1 mM** (●), 0.25 mM (●), 0.5 mM (●), and 2 mM (●) Tz-OMe in 0.5 M TBAPF<sub>6</sub>/MeCN. (G) Plot of discharge capacity versus time m-BE cycling of 1 mM Tz-OMe in **0.5 M** (●), **0.25 M** (●), and **1 M** (●) TBAPF<sub>6</sub>/MeCN.

## PFAS Adsorption

### Synthesis of the adsorbent

List all reagents used, their sources, characterization of raw material (particle size, elemental analysis). Describe the experimental conditions and include photos if helpful. List all reaction and workup conditions used, and any drying or purification methods.

### Characterization of the adsorbent

For insoluble materials, we often rely on elemental analysis; include sample preparation (drying, etc.), raw data for elemental analysis, source (Atlantic Microlab), elemental composition/charge density/functionalization % calculations. Microscopy is also useful for morphology characterization; include instrumentation and parameters used, sample preparation, processing methods, and images. Sometimes spectroscopy can be useful; include any instrumentation and parameters used, sample preparation, processing methods, relevant spectra and images. Other characterizations could include conductometric titrations (list all solutions used, time between points, material preparation (homogenization), charge density calculations).

### PFAS Adsorption Experiments

Describe how adsorbent mixtures were prepared, including solution preparation (homogenization, times for soaking, etc.), and concentration of solutions. Describe the procedure for adsorption experiments and analysis, including prepping LC-MS samples, instrumentation (HPLC-MS, QQQ), method/solvent, parameters (column, flow rate, etc.), QQQ: parent ion masses, product ion masses, collision energies, etc, and blanks with no adsorbent, unfunctionalized adsorbent.

For batch adsorption, include instrumentation used, initial PFAS concentrations, PFAS used, contaminants used (and solution preparation), experimental setup, workup/filtration steps, dilution prior to analysis explanation and calculation, internal standards used and what they 12C PFAS they are used for. Include information on blanks with and without filtration (to verify filter loss, if applicable). Explain how calculations of PFAS removal were performed, any adsorption kinetics calculations, and compare to commercial adsorbents (GAC, IXR), if applicable.

For batch adsorption isotherms, describe the experimental procedure, concentrations of all adsorbent and PFAS, maximum capacity calculations, isotherm assumption (Langmuir or Freundlich).

For column testing, describe the scaling factors used, explanation of scaling factors, instrumentation, values of small-scale column compared to large column, experimental procedure, column volume calculations. Compare to commercial adsorbents (GAC, IXR), if applicable.

Include a general procedure for analyzing PFOS/PFOA solutions in-house, with analysis methods: m/z extracted for PFAS, m/z extracted for standards, elution times, smoothing

For studies performed in real water solutions (feed water, surface water, ground water, etc), include all characterization data on those solutions, including conductivity, dissolved organic carbon/total organic carbon, and pH.

\* Applies to all future papers starting 6/10/26

MS figures will contain processed data while SI figures will contain unprocessed data w/instructions in the SI on how the data was processed

Though we eventually want it labeled with a specific figure #, you should probably start with something you recognize (e.g., notebook page number) so you can order and organize it later.

Results are returned from Atlantic Microlabs as a PDF with columns for elements tested, theoretical mass % of each element, and found mass % of each element. Manually copy “element,” “theory,” and “found” columns into .csv file and label as “element,” “mass % theoretical,” and “mass % experimental” respectively

| <h1 style="margin: 0;">Atlantic Microlab, Inc.</h1>                                                                                               |        |       | Company <input type="checkbox"/> University of Michigan<br>Dept. <input type="checkbox"/> Chemistry<br>Address <input type="checkbox"/> 930 North University Avenue<br>City, State <input type="checkbox"/> Ann Arbor, MI 48109<br>Name <input type="checkbox"/> _____<br>Phone <input type="checkbox"/> (818) 852-0488      Date <input type="text" value="9/26/06"/> |                                    |  |
|---------------------------------------------------------------------------------------------------------------------------------------------------|--------|-------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------|--|
| Sample No. <input type="text" value="AES_11_055_dubing"/>                                                                                         |        |       |                                                                                                                                                                                                                                                                                                                                                                        |                                    |  |
| 6180 Atlantic Blvd. Suite M<br>Norcross, GA 30071<br><a href="http://www.atlanticmicrolab.com">www.atlanticmicrolab.com</a>                       |        |       |                                                                                                                                                                                                                                                                                                                                                                        |                                    |  |
| Professor/Superior: <input type="checkbox"/> Prof. Anna McNeill<br>PGM / CCM: <input type="checkbox"/> 300695195                                  |        |       |                                                                                                                                                                                                                                                                                                                                                                        |                                    |  |
| Element                                                                                                                                           | Theory | Found | Single <input type="checkbox"/>                                                                                                                                                                                                                                                                                                                                        | Duplicate <input type="checkbox"/> |  |
| C                                                                                                                                                 | 38.44  | 60.17 | Elements <input type="checkbox"/> C, H, N, Cl<br>Analysis <input type="checkbox"/> C, H, N, Cl                                                                                                                                                                                                                                                                         |                                    |  |
| H                                                                                                                                                 | 4.84   | 7.38  | Hydrocarbons <input type="checkbox"/> Explosive <input type="checkbox"/><br>M.P. <input type="checkbox"/> 65 °C                                                                                                                                                                                                                                                        |                                    |  |
| N                                                                                                                                                 | 0.00   | 0.0   | Do not subject Yes <input type="checkbox"/> No <input type="checkbox"/> Temp. <input type="checkbox"/> 10 min <input type="checkbox"/> 2 min <input type="checkbox"/> 30 min                                                                                                                                                                                           |                                    |  |
| Cl                                                                                                                                                | 56.72  | 26.84 | Non-hazardous <input type="checkbox"/> <small>Contains no known or suspected hazardous materials as listed in 49 CFR 171.2, 172.101 or 172.102</small><br>Include Email Address or FAX # below<br>aese@umich.edu                                                                                                                                                       |                                    |  |
| Date Received: <input type="text" value="JUN 11 2006"/>                                                                                           |        |       | Date Completed: <input type="text" value="JUN 12 2006"/>                                                                                                                                                                                                                                                                                                               |                                    |  |
| Remark: <input type="checkbox"/> The sample is clean. Please use the attestation card to collect the samples from the donor. They were very much. |        |       |                                                                                                                                                                                                                                                                                                                                                                        |                                    |  |

| element | mass %      |                    |      |                     |        |                       |
|---------|-------------|--------------------|------|---------------------|--------|-----------------------|
|         | theoretical | experimental       |      |                     |        |                       |
|         | PVC         | PVC <sub>37k</sub> | pipe | PVC <sub>pipe</sub> | tubing | PVC <sub>tubing</sub> |
| C       | 38.4        | 38.5               | 37.8 | 38.7                | 53.3   | 38.6                  |
| H       | 4.84        | 4.76               | 4.69 | 4.90                | 6.93   | 4.81                  |
| N       | 0.00        | 0.00               | 0.00 | 0.00                | 0.00   | 0.00                  |
| Cl      | 56.7        | 56.7               | 55.4 | 56.4                | 32.7   | 56.6                  |
| total   | 99.9        | 99.9               | 97.9 | 100                 | 92.9   | 100                   |

Russ will normally send a word doc with the entire HRMS peak list that can just be copy/pasted into an excel sheet. The three columns will be m/z, abundance, abund%

## 46

Process spectrum in MNova. When you are going to export, make sure that your spectrum is fully zoomed out; the only data captured in the next steps is what is visible in the MNova window.

File → Save As → **Script NMR csv (.csv, .txt)** (Script is important because the resulting file is automatically split into two columns by Excel when you open it). Open the csv in Excel. Label the left column “f1 (ppm)” and the right column “Intensity”. You’re done! Copy this into your big Excel sheet.

### GC/MS

Export text file from software. Copy and paste data into your figure CSV file. Label columns as retention time and absolute intensity. Other options could also be relative intensity, or peak area.

### SEC

Export the .txt from the software. Open the file in Excel, copy and then paste the data Title tabs/data/columns according to your detector used, and then retention volume. Examples would be retention volume (mL) and detector response (mV). Common detectors used are UV, RI, or a multi-detector (usually RI and UV).

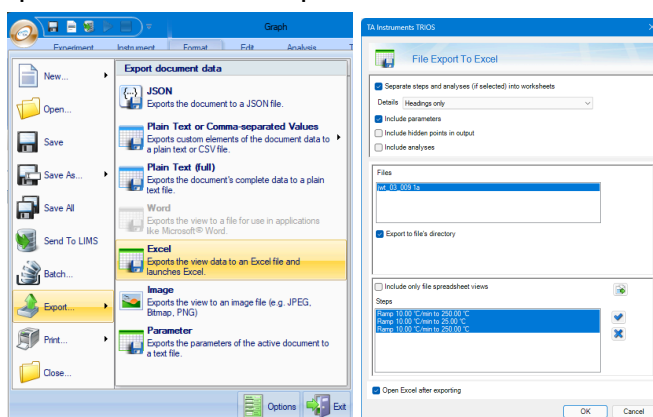
### TGA

Export .txt from software on the computer. Open file in Excel and copy data into your figure .xlsx file. Label columns with relevant titles (typically time (min), temperature (°C), and mass (mg)).

### DSC

#### TRIOS Software

File > Export > Excel. Include parameters.



Open file in Excel. Tabs will auto-populate with data for each temperature ramp and the first tab with information about the full procedure. Each ramp tab will create headings of Time (min), Temperature (°C), and Heat Flow (W/g). These are the un-processed data. (Heat flow

has a parenthetical of “normalized” because it inherently compares heat flow to the mass of sample loaded.)

a.

|   | A          | B                                                                                             | C | D | E | F | G | H | I | J |
|---|------------|-----------------------------------------------------------------------------------------------|---|---|---|---|---|---|---|---|
| 1 | Filename   | JWT_03_009 1A                                                                                 |   |   |   |   |   |   |   |   |
| 2 | Instrument | DSC2A-02608 (192.168.0.126)                                                                   |   |   |   |   |   |   |   |   |
| 3 | Operator   |                                                                                               |   |   |   |   |   |   |   |   |
| 4 | rundate    | #####                                                                                         |   |   |   |   |   |   |   |   |
| 5 | Sample na  | JWT_03_009 1A                                                                                 |   |   |   |   |   |   |   |   |
| 6 | procedure: | Ramp 10.00 °C/min to 250.00 °C; Ramp 10.00 °C/min to 25.00 °C; Ramp 10.00 °C/min to 250.00 °C |   |   |   |   |   |   |   |   |

|    | A                              | B         | C                      | D |
|----|--------------------------------|-----------|------------------------|---|
| 1  | Ramp 10.00 °C/min to 250.00 °C |           |                        |   |
| 2  | Time                           | Temperatu | Heat Flow (Normalized) |   |
| 3  | min                            | °C        | W/g                    |   |
| 4  | 45.01                          | 26.44     | 0.281                  |   |
| 5  | 45.01                          | 26.42     | 0.281                  |   |
| 6  | 45.01                          | 26.39     | 0.281                  |   |
| 7  | 45.01                          | 26.39     | 0.281                  |   |
| 8  | 45.01                          | 26.36     | 0.281                  |   |
| 9  | 45.01                          | 26.35     | 0.281                  |   |
| 10 | 45.01                          | 26.33     | 0.281                  |   |
| 11 | 45.02                          | 26.31     | 0.281                  |   |

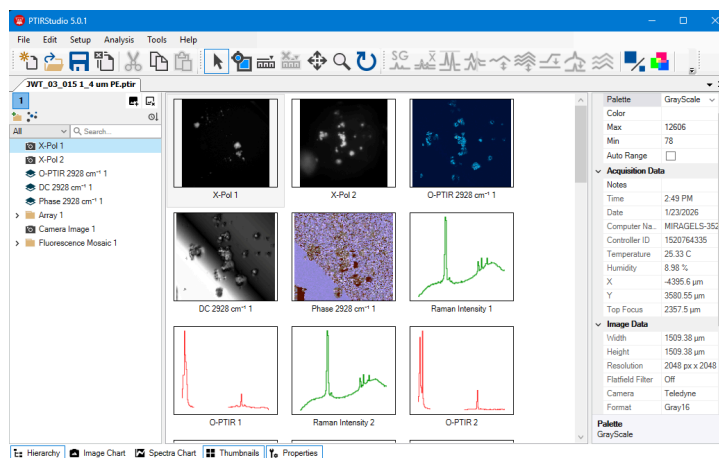
## FTIR

Before taking spectra, go to “Methods” and write down parameters used. After taking spectra, “Export” as a .csv file from dropdown. Note parameters in the .csv. Keep the original .csv file and duplicate for processing

## Raman

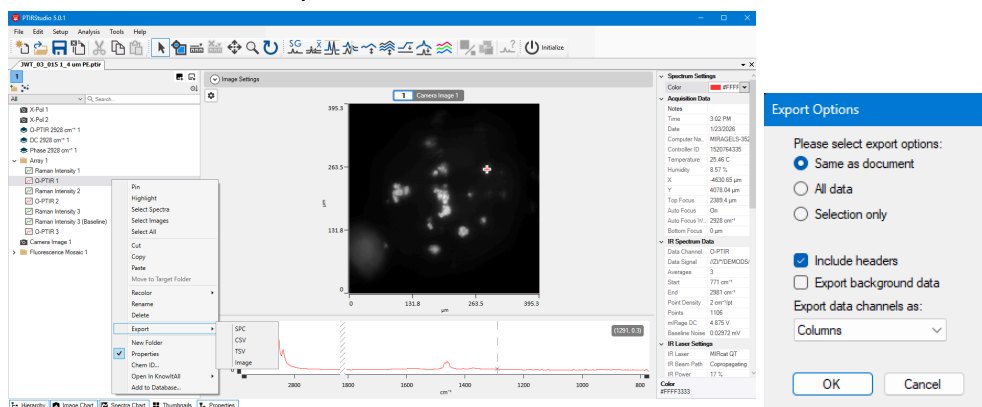
## O-PTIR

When in the main page (Thumbnails) you can view all acquired spectra and images acquired in a particular file. All instrumental parameters will be displayed in a panel on the right.



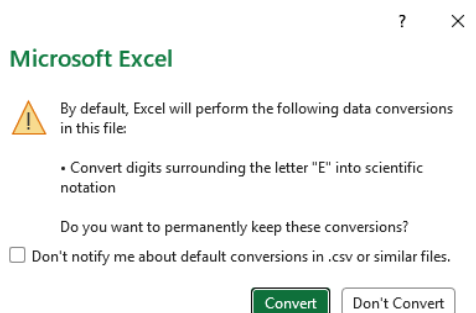
To export a particular spectrum or image, right click the file in the left-hand panel. Depending on what you want to export, you may select to export only the selected

spectrum/image or you may select to export “all data”. Selecting “all data” will export all of that data type (i.e. Raman, PTIR, image) into a combined Excel or as Raw singular images. Select “include headers” and export data channels as “columns”.



When the data exports, it will name the column the same name as is written in the left-hand panel. If you require more detailed naming conventions, I would suggest naming them in the Photothermal software so it will export along with the data. It would likely be useful to choose a convention that allows you to easily correlate spectra with images.

When opening a file in Excel, you will see the prompt: **>Select “Don’t Convert”** Clicking convert will result in your data being truncated and possibly misinterpreted by Excel rather than treating the incoming data as raw text.



When opening in Excel, the file will populate with a label for the file-name of the spectrum from the Photothermal software, but will not include units. >Units for column A should be wavenumber ( $\text{cm}^{-1}$ ) >Units for column B should be O-PTIR Intensity (mV) The units on the y-axis in publications are generally reported as arbitrary units (a.u.) but the instrument reports it in mV.

The two values above the intensity values (-4630.65 and 4078.04) are the location of the acquired spectral data.

|   | A   | B               | C |
|---|-----|-----------------|---|
| 1 |     | O-PTIR 1/O-PTIR |   |
| 2 |     | -4630.65        |   |
| 3 |     | 4078.04         |   |
| 4 | 771 | -0.62155        |   |
| 5 | 773 | -0.63556        |   |
| 6 | 775 | -0.47525        |   |
| 7 | 777 | -0.09996        |   |
| 8 | 779 | 0.07922         |   |

### SEM

Export image from instrument (.jpg or .tiff). Export image parameters/meta data from instrument (beam intensity, beam energy, working distance, etc.)

### EDX

Export project file from TEAM software on the SEM. Open .spc file in the TEAM-adjacent software on the SEM and export the spectrum .csv file. Show both .csv and images of where the spectrum was taken in the source info. Add meta data to source information or SI (working distance, beam intensity, beam energy, etc).

### XPS

### EC lab files

CV- Alt D to copy raw data, paste into excel, make sure units are current vs. Ewe. Denote all electrode materials.

Bulk electrolysis/Batteries- Alt D to copy the raw data, paste in excel, make sure column labels are Ewe (denote reference if applicable) and capacity.

EIS- Alt D to copy raw data, paste in excel, units should be Re(Z)/ohm and -Im(Z)/ohm.

### Conductivity titrations

Write down concentrations/masses of materials used for titrations

Add values for volumes of titrant added and conductivity of the solution at each volume added.

### Flow cytometry/coulter counter

### LC/MS (QTOF and QQQ)

For all LC/MS: note method used, instrument, and meta data in the SI

QTOF: extract area under the curve (make sure the settings are consistent - Integrate method: Agile; Symmetric: 20 ppm)

QQQ: similar to QTOF except use the agilent quantitative analysis software on the instrument, used a made method (explain method in SI) for integrating peaks, and export the tables/peak areas into source data

# Presentations

## How to write a conference abstract

The following advice was originally excerpted (and edited) from [“How to write a scientific abstract in six easy steps”](#) and then revised over many years by the McNeil Group.

1. **Topic & Challenge Statements.** First sentence: What’s the topic and why is it important? Phrase it in a way that your reader will understand. The readers are likely chemists, so they know the basics, but will want to know specifically what topic your paper/presentation covers. Second sentence: State the problem you tackle. What’s the key research question? If you can’t summarize the gap/challenge in one key question, then you haven’t focused it down to the essential question yet. Keep working at this step until you have a single, concise (and understandable) question.
2. **Explain, in one sentence, how you tackled the research question.** What’s your big new idea or approach? What is the rationale behind it/why do you think it will solve this problem or fill this gap? This sentence should be general and not too detailed (yet).
3. **In one sentence, what did you actually do to answer/address the research question.** Did you run experiments? This is likely to be the longest sentence, but don’t overdo it - we’re still looking for a sentence that you could read aloud without having to stop for breath. Remember, the word ‘abstract’ means a summary of the main ideas with most of the detail left out.
4. **In one sentence, what are the most important results that came from the work?** Hint: These results should directly address that research question/gap you mentioned above. Don’t tell us about all the results, just the most significant one(s). As much as possible, provide some context – how do these results compare to others in the field?
5. **As a single sentence, what’s the key impact of your research?** Here we’re looking for a summary of the implications on the field/others. Why should other people care? What can they do with your research?