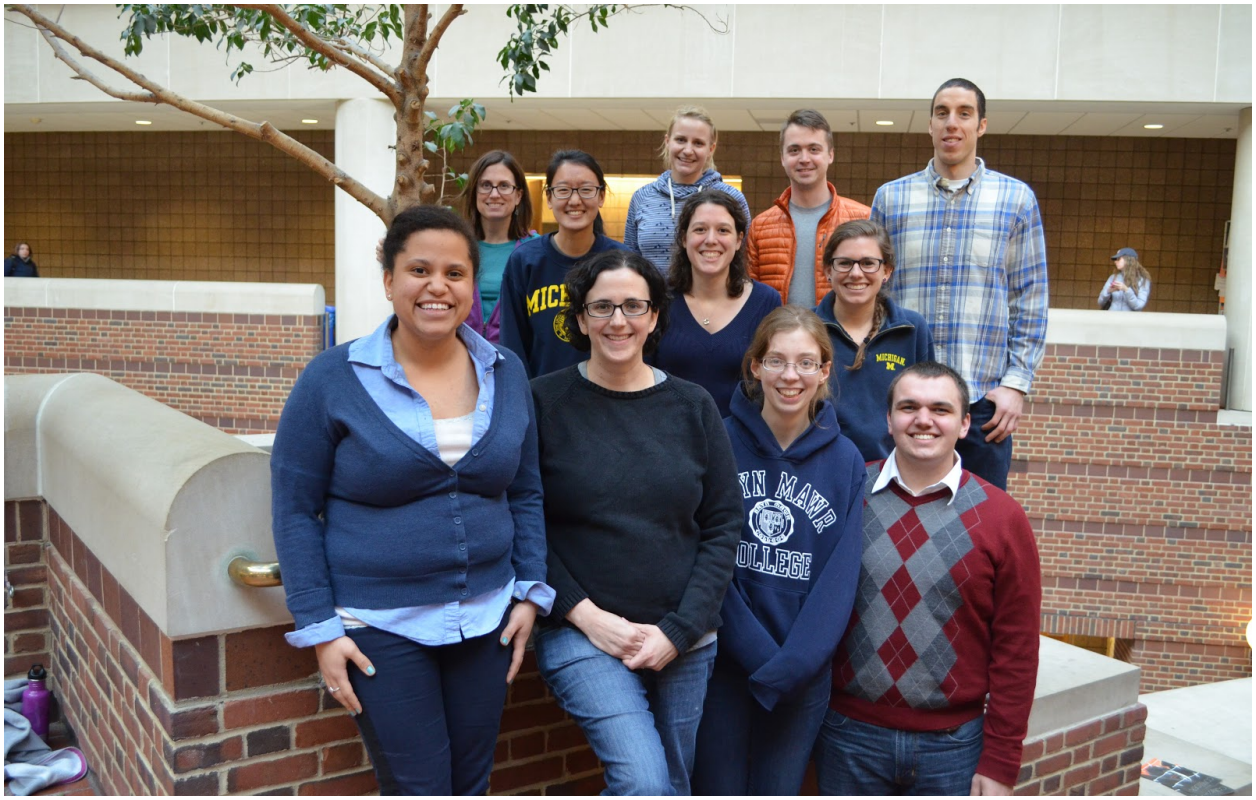
McNeil Group Handbook

Policies, Procedures and Guidelines



Last Updated: June 2015

www.umich.edu/~michchem/faculty/mcneil/index.html

http://www.umich.edu/~ajmlab/

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Lab Safety

General

- Make sure you complete the UM-OSHA Comprehensive Laboratory Safety Training course (www.osehtraining.umich.edu/osehtraining) and read the Chemistry Department Safety Manual before initiating research. Provide a copy of your completion certificate to the group safety officer and Prof. McNeil.

- 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 Prof. McNeil before beginning research.

- Notify the group safety officers (Amanda and/or Pete) 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 Prof. McNeil. Open-toed shoes and shorts/skirts (without leggings) cannot be worn in the lab.

- For additional safety resources, please consult the "safety information" section of the group website.

Guidelines for a Safe Working Area

Bench and Hood Area

- Your workspace cannot 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_2 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 Space

- 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** or **Tracy Stevenson** (Departmental Lab Safety) at **734-764-7316** or **steventi@umich.edu**.

Lab Safety Checklist

Please complete the following checklist with the group safety officer, and return a signed, scanned copy as a pdf file to Prof. McNeil before beginning to work in the lab.

- ❑ I have received safety glasses and a lab coat and agree to wear them at all times when in lab. I am aware of acceptable clothing to wear in lab.

- ❑ I am aware of the location and operation of the safety shower, eye-wash, fire extinguisher, blast shield, and fire alarm in ALL of the group laboratory rooms.

- ❑ I am aware of the University of Michigan chemical hygiene plan and the group-specific hygiene plan, and have read and signed all lab-specific SOPs and I have become familiarized with their contents.

- ❑ I have completed the OSHA safety training.

- ❑ I am aware of emergency phone numbers and department contact numbers in the event of an accident, chemical spill, or other emergency.

- ❑ I know how to access MSDS (material safety data sheets), and I will refer to these if I have any questions about the safe handling of any reagent.

- ❑ I have received a lab notebook and I am aware of the correct protocols for keeping complete and accurate records of my research.

- ❑ I will conduct my research with honesty and integrity and will not intentionally fabricate or misrepresent any scientific data.

- ❑ I have viewed the group job list and will consult the appropriate person before using any equipment for which I have not yet received proper training.

- ❑ 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 will be properly trained (i.e., read the SOP and talk to an experienced user) before handling any pyrophoric compounds.
- ❑ I will seek advice from experienced group members about all new procedures, and I will consult with Prof. McNeil if any procedure poses a potential safety concern.

- ❑ I will consult with Prof. McNeil 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 Prof. McNeil if the problem persists or is repeated.

- ❑ I agree to all of the above items.

_____	_____	_____
Name (printed)	Name (signed)	Date

General Group Policies

Supporting Information

This document is an incredibly important document and one that should replicate the results you obtained as depicted exactly in your lab notebook. Every section of SI should be associated with it a page from your notebook and data files. Please see examples from our group's recent publications for guidance on how to prepare the SI. The group policy is that you must provide (as a PDF file) the scanned notebook pages that correspond to the procedures in the Supporting Information. In addition, you will also provide scanned original copies of the ^{1}H and ^{13}C NMR spectra, as well as the HRMS results, elemental results, rate profiles, GPC data etc. Your SI must conform to the above criteria or you will be asked to re-run the experiment again prior to submission.

Group Collaborations

Collaborations are a vital part of the scientific enterprise. When you agree to engage in a collaborative project, you are committing to providing the collaborator with the highest quality material, no matter how much time it takes. Your collaborative partner will spend a significant time working with the material you provided them. The group policy is that with each sample you must provide (as a PDF file) the scanned notebook page that corresponds to the exact procedure used to make the sample, the ^{1}H NMR spectrum of that sample, the yield and estimated purity, and any other relevant characterization data (e.g., the GPC for polymers or elemental analysis for Ni complexes). You must conform to the above criteria or you will be removed from the collaborative project, and if your funding is related to this project, you will have your position changed from GSRA to GSI.

Group Meetings

Research group meetings occur every week. The format rotates between (i) ASAP highlights, (ii) critique of a recent paper, (iii) subgroup (see below), and (iv) formal research presentations. Please make copies of slides for all group members prior to the meeting. See website for schedule.

Subgroup Meetings

Each member provides a brief update on their progress (15 min) and gets feedback and suggestions from other group members. Each student should prepare their presentation following the guidelines outlined in the shared Google sheet.

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 8 h per credit hour. They can only perform research if a graduate student or post-doc is also in lab. The undergraduates are expected to attend and participate in all group meetings.

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 Anne, and *therefore must be approved by Anne prior to their presentation.*

Expectations and Vacation Time

Group members are expected to work at least 60 h/week, including one day on the weekend.

Each student/post-doc is allotted 21 days of vacation per calendar year (Jan-Dec). This includes UM holidays (e.g., Thanksgiving day). You are expected to work 6 days a week. So if you work less than that, you must use a vacation day. To keep track of everyone's dates, there is shared Google calendar. You must write your initials on the date(s) you will be taking off AND what vacation day that is for you (e.g., 10/21).

Searching and Reading the Literature

Searching the past literature

SciFinder Scholar

This program should be installed on your personal computer and used whenever you want to find out how to do a specific synthetic transformation. For more information, refer to "Information Retrieval: SciFinder and SciFinder Scholar" by Damon D. Ridley, Wiley, 2002.

ISI Web of Science

There are several very useful functions of this website.

A. Cited Articles Search

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

B. General Topic Search

Use the "and" command to link two concepts and use "*" to expand. For example, if you want to search for fluorescent polymers, but also want to include any search where "fluorescence" is also used. Your search command would read "fluor* and polymer."

C. 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.)

Reading the Current Literature

Keeping up with the current literature is essential to becoming an independent and successful scientist. You should dedicate several hours per week to browsing the latest issues of key journals (to gain breadth) and reading the important articles in your field (to gain depth). My advice is to sign-up for receiving the latest articles either via email or RSS feeds. Personally, I use Feedly to aggregate all my RSS feeds and read them on Reeder 2. I then email myself the notable articles and move the PDF into Mendeley (if warranted) later.

More Suggested Reading Material

“Alternative Careers in Science: Leaving the Ivory Tower” by Cynthia Robbins-Roth

“A PhD is Not Enough: A Guide to Survival in Science” by Peter J. Feibelman

“Tomorrow's Professor: Preparing for Careers in Science and Engineering” by Richard M. Reis

“The Academic Job Search Handbook” by Mary Morris Heiberger

“At the Bench: A Laboratory Navigator” by Kathy Barker

Lab Notebook Guidelines

General

- Every experiment you do MUST be accompanied by an entry in your lab notebook.

- Every experiment you report in SI MUST be accompanied by an entry in your lab notebook.

- Only use the standard lab notebooks provided for you. Do not remove any pages. Label your notebook with your initials. Your first notebook is "a" or "I." For example, Anne's first notebook is AJM_A or AJM_I.

- If you repeat a procedure, record it as a new experiment with its own page and refer to the previous page for the procedure. However you MUST record the quantities of starting materials and yields for products in the new experiment, even if it is identical. If anything else is different, workup conditions, chromatography conditions, etc, record these changes as well.

- Only use pen (non-erasable ink) and do not scribble or scratch out anything in your notebook. Do not use whiteout. If there is a mistake, use a single line through the mistake.

- Make sure you date your experiments, including the year. Also 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 for each entry.

- 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 (The product was purified by column chromatography.)

- When you are determining the mass of product obtained, record the mass based on the accuracy of the balance.

- If the NMR spectrum is impure and you have to re-purify, report a new yield on the same page that corresponds to the purified product. For the supporting

information, you should report the yield that matches the final, pure product, not a previous impure fraction.

- Indicate in your notebook the spectra name and date acquired for all data relating to that experiment.

- 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. If you prefer, you can have two columns in your notebook – one listing the amount you plan to add and one listing the amount you actually add. But you MUST have the amount you actually added, as well as calculations that match the moles, equivalents, etc of the other reagents.

- If you decide that for one reason or another you don't think the data obtained is valid, note this in your notebook and state your reasoning. For example, "There was significant quenching of the monomer during the polymerization as evidenced by the IR signal corresponding to this by-product."

- Draw a single, diagonal line through the blank space on any page once you have finished the experiment so that future modifications cannot be made.

- Read pages 92-98 in the "At the Bench" laboratory manual located in our group library.

Table of Contents

- Save the first 10 pages of your lab notebook for a Table of Contents.

- Write a generic reaction scheme and record the page number(s) for each experiment.

- Update the TOC weekly!

Summary

Ultimately, your 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!**

Collecting and Archiving Scientific Data

Uncertainty in Measurements – Significant Figures

All measurements have some level of uncertainty. Significant figures include all the digits you are certain about PLUS one additional uncertain digit. See attached discussion. Note that our balances are uncertain in the *last* digit you can read.

Counting Significant Figures

Leading zeros are not significant. 0.008 has one significant figure
Captive zeros are significant. 1.02 has three significant figures
Trailing zeros are significant. 40.00 has four significant figures

Rules for Rounding

In a series of calculations, carry the extra digits through to the final result and then round. If the digit to be removed is less than 5, the preceding digit does not change. (1.33 = 1.3) If the digit to be removed is greater than 5, the preceding digit goes up by one. (1.36 = 1.4) Only look at the first number to the right of the significant figure. (4.348 = 4.3) If the digit is 5, then round to the closest number. (1.35 = 1.4 and 1.75 = 1.7)

Calculations and Significant Figures

For multiplication and division, the answer should have the same number of significant figures as the least precise measurement. (4.56 x 1.4 = 6.4)
For addition or subtraction, the answer should have the same number of decimal places as the least precise measurement. (12.1 + 18.0 + 1.103 = 31.1)

Data Collection

Save all spectra and original data labeled with an identifier that corresponds to the page number in your notebook. Indicate in your notebook the spectra name and date acquired. Be prepared to show this data to me OR a reviewer when asked. We should

also be able to find this data after you have graduated so save your files in an organized manner.

Labeling and Storing Compounds

- 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. Sharpie's do not last the test of time!

- Store all synthesized materials in small disposable vials with screwcaps. Do not store any compound in an expensive flask with ground glass joints!

- Indicate the amount of material inside the vial on the screwcap (e.g., 52 mg).

- Store all synthesized compounds either near your bench or in your assigned shared refrigerator. Do not store your compounds on the group chemical cabinets or in the group refrigerator.

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. See also, senior members of our research group.

- 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 (see below). You can supplement TLC with GC analysis, crude NMR spectra, and IR. None of these techniques are a substitute for TLC.

- Always work up reactions immediately upon completion.

- Take the time to identify by-products the first time through a synthesis.

TLC and Flash Chromatography

Adapted from Prof. David B. Collum's "Mother Liquor Lecture" Cornell

TLC

1. Monitor all reactions before adding the last reagent, during the reaction, and after the quench. If something goes wrong, you will not know when that happens unless you are monitoring the reaction!

2. Always co-spot the reaction mixture with the starting materials to aid identification.

3. If two spots are extremely close, then spot them twice (see picture). If a Z pattern develops, they are NOT the same material. **insert image**

4. Visualization: (1) By sight! (2) UV (3) Stains (see next page).

5. For amines, add 0.5% Et3N to the solvent chamber. For acids, add 0.5% HOAc.

6. Draw the TLC plate in your notebook and mark with observations.

Flash Chromatography

Still, W. C.; Kahn, M.; Mitra, A. "Rapid Chromatographic Technique for Preparative Separations with Moderate Resolution." *J. Org. Chem.* **1978**, *43*, 2923-2925.

1. Pick a favorite solvent pair (e.g., EtOAc/hexanes) and get to know it in all ratios.

2. Pack column under positive pressure.

3. For many samples, it is convenient to first add silica gel (about 1 scoop per 250 mg) and concentrate to form a coated powder. Add this solid to the pre-packed column and then add the sand.

4. Elute at 2"/min. Change to more polar solvents over time if needed.

5. Monitor the progress of the column by TLC in real-time!

6. Use half TLC plate to spot 5 test tubes, run TLC and then flip over and use the other half for another 5 test tubes.

7. For small-scale reactions, a pipette can serve as a column.

8. OR - Use the automated chromatography system in the lab to run simple columns much faster!

TLC Stains

(Adapted from Prof. Justin DuBois, Stanford University)

Anisaldehyde

Add 2.5 mL of AcOH and 6.5 mL of p-Anisaldehyde to 300 mL of ice cold 95% EtOH (or EtOAc, not denatured EtOH). Cautiously add 8.5 mL of concentrated H_2SO_4 dropwise over 60 minutes. Store unused portions in freezer.

CAM (Ceric Ammonium Molybdate)

4 g	Cerium sulfate (complex with H2SO4)
100 g	Ammonium molybdate tetrahydrate
900 mL	deionized H_2O
100 mL	conc. H_2SO_4

Potassium Permanganate

2 g	$KMnO_4$
20 g	K_2CO_3
5 mL	5% NaOH

Dissolve KMnO4 in 300 mL water.
Add K_2CO_3 followed by NaOH.

Iodine

Add 500 mg I_2 to 20 g silica gel in amber jar.

Ninhydrin

3 g	Ninhydrin
30 mL	glacial acetic acid
970 mL	n-butanol

Stir until dissolved. Store in a brown bottle in the freezer.

PMA (Phosphomolybdic acid)

100 g	PMA
1273 mL	95 % ethanol

Stir until dissolved. Store in freezer.

Searching the Inventory

All chemicals in the McNeil lab are organized in Vertere. This system records information on all chemicals at the University of Michigan. Access to Vertere requires a university internet connection using the following URL.

Vertere can be accessed through a secured login using either the [1] McNeil group account (ask a group member for username and password), or [2] a personal account. To obtain a personal account, contact Anson Pesek (ahpesek@umich.edu).

Logging in with the McNeil group account

The McNeil group account is authorized to transfer chemicals between locations on the Vertere website. Therefore, only chemicals that belong to the McNeil lab are visible on this account.

To perform a search of McNeil lab chemicals:

1. Click **Chemicals** in the middle of the page
2. Click **View/Edit**
3. Search for chemicals in one of two ways

    a. View entire inventory

Do not input any information and press **enter** on your keyboard (or click the **Search** button on the far right). All of the chemicals in the McNeil lab inventory will be included in your results.

    b. Specific search

To find the location of a specific *chemical bottle*, the barcode # should be used.

To find the location of a specific *chemical*, enter in the CAS number.

4. Browse through all of your search results by clicking **View All**.

5. Chemicals may be sorted by location, barcode (highest #s are most recent), name, etc.

> Results will display the most updated inventory, so interpret them accordingly. Newly ordered chemicals will appear the *day* they are received by the CHEM building. Used (empty) chemicals are removed from the system within *1 or 2 months*.

6. Log out immediately after use by clicking the **logout** icon on the top right of the sheet. Only 5 users can access Vertere in the entire U of M, so improper or delayed logouts mean other people cannot access the system.

Logging in with a personal account

These accounts can view all chemicals within the university system, but cannot make any changes to the information listed. To find a chemical in another lab, follow the above instructions to do a specific search (3b) for the desired chemical. Write down all available information before visiting a lab to borrow any items.

Chemical Organization – in Vertere

Each room and closet of the McNeil lab appears as a separate location in Vertere. Each room is further split up into sub-locations, which identify the specific location of each chemical. Note that the first four digits correspond to the room number, 2621, and the sub-location is identified as *Bromides*.

While nearly all chemicals stored in 2621 are organized by functional group, some chemicals are sorted strictly by location. Chemicals are sorted in the following order (1→3 then a→z)

1. Storage Necessity. Store chemicals at low T or in a air/moisture-free atmosphere as required.

Air/moisture-free locations: 2621-Glovebox 1 [G1], 2621-Glovebox 2 [G2], 2623-Dessicator [DE]

Low T locations: 2615-Refrigerator A [A] or B [B], 2621-Freezer [Fr], 2623-Refrigerator C [C] or D [D], 2629 – Refrigerator E [E] or F [F]

2. Price/Scarcity. Chemicals that cost >$400/g should only be handled by those whom they were specifically ordered for, and assigned to the nearest refrigerator.

3. Functional Group.

- Transition metals and lanthanides: 2615-Transition Metals [T]
- Acids: 2615-Nitric Acid [N], 2621-Bases [Ba], 2623-Acetic Acid [Ac], 2623-Organic Acid [O], 2623-Inorganic Acid [I]
- Halogen, non-metal, and semi-metal/metalloid compounds: Chemical cabinet in 2621 (see next section)
- Main-group metals: 2623-Main-Group Metals [M]
- Alkali metals, alkaline earth, and basic/poor metals

Chemical Organization – in 2621

1. Chemicals are first sorted by lowest number functional group (AA, 1-23) (i.e., 4-Hydroxy-3-methoxybenzaldehyde is sorted as an aldehyde, 11) Functional groups may occupy an entire shelf or a *section* within that shelf.

2. Sub-categories (a, b, or c) are arranged within a section from left to right (i.e., 9a to 9b). Sections are further organized (left to right) from aromatic to alkyl to pure functional group (i.e., PhBr to BrC_6H_{13} to Br_2). Larger/longer aromatic/alkyl groups will be on the left of each section (i.e., $BrC_{10}H_{21}$ to BrC_6H_{13}).

Further Notes

- All S, Se, etc. derivatives should be organized according to the O parent compound
- Heteroaromatics (i.e., furan) are NOT sorted by their characteristic functional group (i.e., ether, 15), but by the substituents (i.e., 2-bromofuran is in bromide, 19). Only carbon substituted or non-substituted derivatives should be labelled as heteroaromatics, 20.
- Conventional polymers like poly(ethylene) are labeled "2". Polymeric forms of a reactive compound (i.e., paraformaldehyde) are organized according to the deliverable functional unit (i.e., formaldehyde, 11)
- If you are unsure where a new chemical should go, file it as misc. (23) and the inventory manager can decide.

Incoming Chemicals

The future location of a chemical must be identified *before* it is ordered. Locations are identified by the letter in brackets (mentioned above) or the priority number listed for 2621. Delivered chemicals should be placed in the green Akro bin next to the GC in 2621. The inventory manager will gather the chemicals daily, then write the location letter/number in big letters on the bottle and cap, as well as placing the barcode on the chemical. Chemicals will be delivered to the bench of the person that ordered them.

Maintaining the Inventory

All chemicals in circulation should have a barcode and large letters/numbers on them. Any chemicals without such markings have not been properly inventoried, and should be given to the inventory manager immediately.

Chemicals may be moved temporarily from their group location for personal use. Non-group members must completely fill out the sign-out sheet located on the side of the 2621 chemical cabinet. Borrowed chemicals will be tracked down during each group clean-up, so a clear indication that the chemical has been returned is helpful to

all parties. If a group member chooses to store a chemical for >2 weeks, a “McNeil group only” sign-out sheet located on the side of the 2621 chemical cabinet should be used.

Permanent changes in the location of a chemical should ONLY be performed by the inventory manager.

Outgoing (empty) Chemicals

Clipboards are posted within each synthetic lab where barcode stickers should be placed. These are removed monthly by the group safety officer, and subsequently deleted from the inventory.

Org. Chart for 2621 Chemicals

Priority (Descending order)	2621 Label	Functional group	Formula	Prefix	Suffix
AA	Amino Acid	Amino acid			
1	Deuterium	deuterium	-D	deutero-	
2	Polymer		$(x)_n$		
3	Silicon		Si		
4	Boron		B		
5	Phosphorous		P		
6	Ammonium Salts	Ammonium	NH_4^+	ammonio-	-ammonium
7a	Carboxylic Acids	Carboxylic acids	-COOH	carboxy-	-oic acid
7b	Sulfon-	Sulfonic or Sulfinic groups	$-SO_3R$ $-SO_2R$	sulfo- sulfino-	-sulfonic acid -sulfinic acid
8	Esters	a) Acid Anhydride b) Esters c) Acyl halides	-COOCO -COOR -COX	R-oxycarbonyl - halocarbonyl-	-oic anhydride -R-oate -oyl halide
9	Amides	a) Amides b) Imides or Amidines	$-CONH_2$ -CON=C< $-C(=NH)NH_2$	carbamoyl- imido- amidino-	-amide -imide -amidine
10	Nitrile	a) Nitriles b) Nitro or Isocyanide	-CN $-NO_2$ -NC	cyano- nitro- isocyano-	-nitrile isocyanide
11	Aldehydes	Aldehydes	-CHO	formyl-	-al
12	Ketone	Ketones	=O	Oxo-	-one
13	Alcohols	Alcohols b)peroxides	-OH -OOH	hydroxy- peroxo-	-ol
14	Amines	a)Amines b) Imines or Hydrazine	$-NH_2$ =NH $-NHNH_2$	amino- imino- hydrazino-	-amine -imine -hydrazine
15	Ether	Ether	-C-O-C	Alkoxy-	Ether

16	Chloride	Halide	-Cl	Chloro	
17	Fluoride		-F	Fluoro	
18	Iodide		-I	Iodo	
19	Bromide		-Br	Bromo	
20	Heteroaromatic				
21	Aromatic		(4n+2) e-		
22	Hydrocarbon	Saturated Unsaturated	$-C_nH_{(2n+2)}$		
23	Misc.	All others			

Ordering Chemicals and Supplies

If the chemicals you need are located in the building, then you should make an effort to retrieve them and use them. If this is a reaction that you are going to be doing often, on large scale, or the reagents are very expensive, then we can order our own. But I always prefer you try it first using the chemicals in the building. I want to avoid ordering chemicals that we use once (or twice) and then never again.

To order a chemical, determine what purity you need. For example, does it need to be dry or is it cheaper to distill/sublime? Find the best TWO vendors/prices for the quantity you need. This can be done in one of two ways-for Aldrich, Fisher/Acros and VWR please use Wolverine Access--Marketsite to find the UM pricing. For all other supplies use SciFInder Scholar—see specific instructions below. Enter this information in the McNeil orders spreadsheets.

Check all closets and labs for the supplies before ordering new ones. If we are out of a specific item, check the inventory list for each closet for supplies to identify the appropriate catalog number and enter it into the McNeil orders spreadsheet. Broken glassware should be fixed rather than replaced. Check the group supply of glassware for unusual or rarely used items.

1) Identify a vendor (2 vendors for chemicals). For most previously ordered lab supplies and chemicals, previously used vendors can be found in the shared Google doc as a starting point. Prices and catalog numbers can change, so always double check this information before you copy and paste. One can search for chemical vendors (by CAS # or structure) using SciFinder or Reaxys, or the following website: http://www.emolecules.com/ which is operated by Reaxys.

2) Fisher*, Aldrich, VWR, OfficeMax and CGI (gases) are all hosted through Marketsite. Please **always** look up prices and catalog numbers for these vendors through Marketsite because prices on public websites are different from UM prices, and some supplies that are listed publicly are not available through Marketsite, meaning we **cannot** order them. *When searching for vendors, be aware that many, including Acros, Alfa Aesar, Oakwood, Encompass, Maybridge, and ChemGlass should be ordered through Fisher. *If you want a chemical from one of these vendors, look it up in **Fisher** using Marketsite and*

*use that price and catalog number, **not** the information you find using Reaxys, Scifinder or Emolecules.*

3) To access Marketsite, use the following steps:
    i) Go to the "Faculty & Staff" tab in Wolverine Access
    ii) Click "M-Marketsite Browse Only"
    iii) Click on vendor names and find the relevant information

4) Once you have the necessary information, enter it into the appropriate Google doc (chemicals or supplies). Include two vendors for chemicals.

5) Special cases and exceptions:
    - If only one vendor sells a chemical, then you don't have to list two.
    - We have special quotes for commonly used regular and deuterated solvents—for these, only the name needs to be listed. Solvents should be put on the order sheet when the last keg or bottled is **opened**, **not** after it has been fully consumed.
    - **If you need something especially expensive, especially if ordering a large amount, contact the sales rep for the company and request a discounted quote.**

Cold Bath Temperature Chart

System	°C	System	°C
p-Xylene/N_2	13	Carbitol acetate/CO_2	-67
p-Dioxane/N_2	12	t-Butyl amine/N_2	-68
Cyclohexane/N_2	6	Ethanol/CO_2	-72
Benzene/N_2	5	Trichloroethylene/N_2	-73
Formamide/N_2	2	Butyl acetate/N_2	-77
Aniline/N_2	-6	Acetone/CO_2	-77
Cycloheptane/N_2	-12	Isoamyl acetate/N_2	-79
Benzonitrile/N_2	-13	Acrylonitrile/N_2	-82
Ethylene glycol/CO_2	-15	Sulfur dioxide/CO_2	-82
o-Dichlorobenzene/N_2	-18	Ethyl acetate/N_2	-84
Tetrachloroethane/N_2	-22	Ethyl methyl ketone/N_2	-86
Carbon tetrachloride/N_2	-23	Acrolein/N_2	-88
Carbon tetrachloride/CO_2	-23	Nitroethane/N_2	-90
m-Dichlorobenzene/N_2	-25	Heptane/N_2	-91
Nitromethane/N_2	-29	Cyclopentane/N_2	-93
o-Xylene/N_2	-29	Hexane/N_2	-94
Bromobenzene/N_2	-30	Toluene/N_2	-95
Iodobenzene/N_2	-31	Methanol/N_2	-98
Thiophene/N_2	-38	Diethyl ether/CO_2	-100
3-Heptanone/CO_2	-38	n-Propyl iodide/N_2	-101
Acetonitrile/N_2	-41	n-Butyl iodide/N_2	-103
Pyridine/N_2	-42	Cyclohexene/N_2	-104
Acetonitrile/CO_2	-42	Isooctane/N_2	-107
Chlorobenzene/N_2	-45	Ethyl iodide/N_2	-109
Cyclohexanone/CO_2	-46	Carbon disulfide/N_2	-110
m-Xylene/N_2	-47	Butyl bromide/N_2	-112
n-Butyl amine/N_2	-50	Ethyl bromide/N_2	-115
Diethyl carbitol/CO_2	-52	Acetaldehyde/N_2	-124
n-Octane/N_2	-56	Methyl cyclohexane/N_2	-126
Chloroform/CO_2	-61 (-77)	n-Pentane/N_2	-131
Chloroform/N_2	-63	1,5-Hexadiene/N_2	-141
Methyl iodide/N_2	-66	i-Pentane/N_2	-160