

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] Vertere editor account, or [2] a personal account. To obtain a personal account, contact Anson Pesek (ahpesek@umich.edu).

Logging in with the McNeil group editor 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 BrC₆H₁₃ to Br₂). Larger/longer aromatic/alkyl groups will be on the left of each section (i.e., BrC₁₀H₂₁ to BrC₆H₁₃).

Further Notes

- All S, Se, etc. derivatives should be organized according to the O parent compound. Disulfides are on the misc. shelf.
- 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. The inventory manager will gather the chemicals daily, then write the location letter/number in big letters on the bottle and cap. Chemicals will be delivered to the bench of the person that ordered them. That person is responsible for putting the barcodes on the vials.

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.

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

Outgoing (empty) Chemicals

Clipboards are posted within the labs 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 ₃ R -SO ₂ R	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 _n H _(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 McNeil orders spreadsheet to identify the appropriate catalog number and re-enter it in a new row. 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 sheet (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, copy the relevant info from the “frequently ordered items” tab into the main sheet. 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.