

# User's Manual For HERMAN

## Version 0.1

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# Chapter 1

## Overview of HERMAN

HERMAN is a customized Freeslate CM3 (now known as the Unchained Labs Freeslate) equipped with sufficient tools to process many synthesis workflows. These include tools for dispensing solids and liquids, capping and uncapping of vials, centrifugation, sonication, heating, stirring, and cooling.

The general procedure for using HERMAN is to:

1. Specify your synthetic protocol by designing a “Library” in Library Studio (Chapter 2).
2. Set up the robot deck with all of the tools, parts, and compounds needed for your protocol (Chapter 3)
3. Use Automation Studio to run the “Sample Preparation” protocol, which executes your library (Chapter 4).

If you have any questions, comments, suggestions, or other notes about this manual, please contact the author. As this is a bespoke instrument, all of the documentation is a work in progress and any suggestions are greatly appreciated.

### 1.1 Deck Elements



Working left to right, Herman contains:

- A waste bin
- Deck 1–2: a tip rack position, SV hopper positions, and positions for the SV tool/classic dispense head, and the PDT tools
- Deck 3: a liquid waste disposal and sample vial rack
- Deck 4–7: a balance with integrated draft shield
- Deck 8–9: tip rack positions

- Deck 10–11: a heat/cool/stir bay, and two heat/stir bays
- Deck 12–13: three heat/stir bays
- Deck 14–17: empty space
- Deck 18–20: a storage hotel for plates, tip racks, and solvent reservoirs
- Off-deck 1–2: a sonicator, blotting station, and air knife
- Off-deck 3–4: capping station and two substrate positions
- Off-deck (not shown): centrifuge

Each of these elements is designed to work with a standardized SBS-format footprint (i.e. 96-well plates). **The various tools, parts, and consumables associated with the instrument are specifically chosen: always use the ones provided, or contact the maintainers if you want to use something which is not specified here!**

## Chapter 2

# Designing Your Experiment

Most experiments can be described as some mixture of solid and liquid additions and removals, with some mixing, stirring, and heating. In this Chapter you will learn how to program your experiment. The goal of creating a Design is that every step of your process is recorded for later reference, and so any data you generate can be associated with the original design parameters.

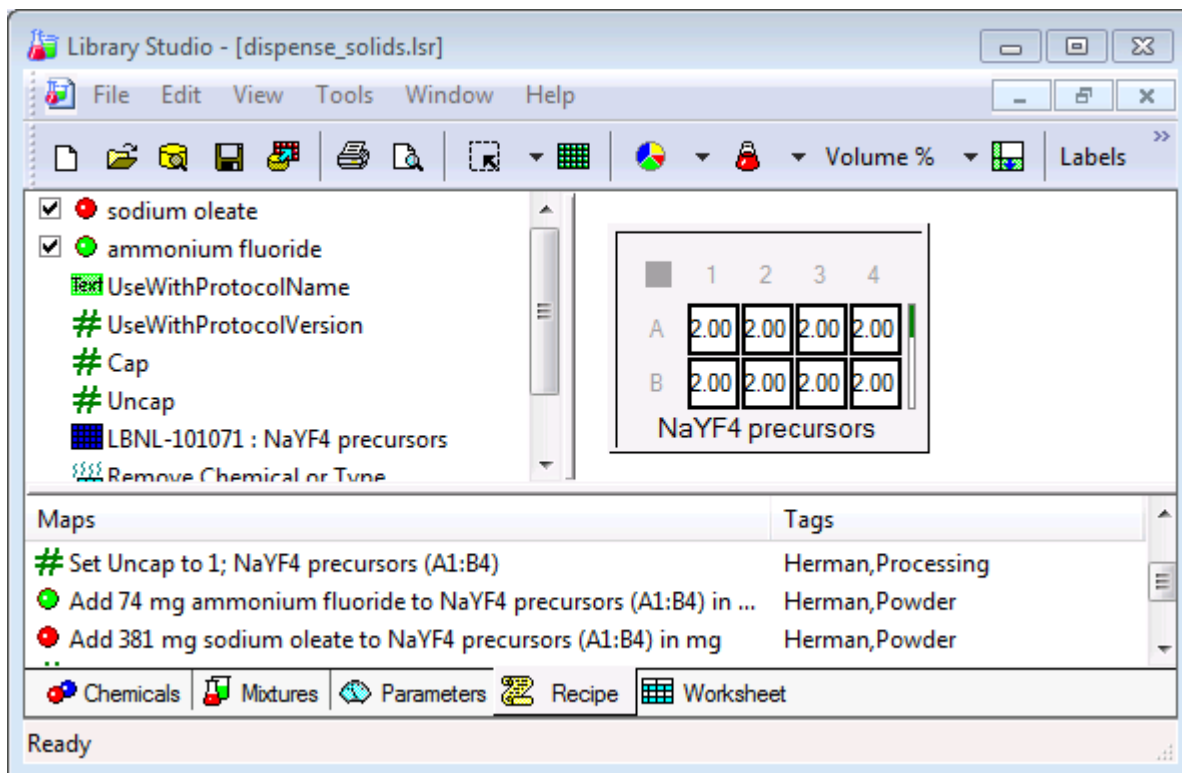
To help you get started, on the HERMAN computer you will find some useful templates in **My Documents ▶ library\_templates**. You can also open existing designs from the database (e.g. LBNL-1051 is a CdSe synthesis). Basing your design off of these starting points will help you avoid many of the common pitfalls.

If you plan to use HERMAN to prepare reaction vessels for use in WANDA, you should read the WANDA manual to learn about the instructions specific to that instrument. A good starting point is design 1051 from the database.

## 2.1 Step-By-Step Instructions For Creating a Design







1. We create our Designs using the program **Library Studio**. Open **Library Studio** on the HERMAN computer by clicking on the taskbar icon, or selecting it from the Start Menu.
2. Open a template using **File/Open/From File...**, from the folder **My Documents\library\_templates**. The file **main\_template.lsr** is a good example.
  - Alternately, you can open a design from the database using **File/Open/From Database**. Design 1056 is a good example of reagent dispensing, and 1051 is a good example of using Herman and Wanda together.
3. You should now see a screen that looks something like this:



4. We will start by noting the chemicals you plan to use in your experiment. These are divided into individual compounds and chemicals (**Chemicals**) and mixtures of compounds (**Mixtures**). For compounds like sodium chloride, use **Chemicals**, but for sodium chloride solution in water, use **Mixtures**.
5. In the **Chemicals** tab, enter the names of the chemicals you are going to use, in lowercase.
  - If you want to dispense by mol, enter the molecular weight (MW) of your compound.
  - If you want to dispense a liquid by mass, enter its density.


Once finished, your chemicals list should look something like:



	Color	Name	MW	Density
1		flour		
2		sodium chloride	58.440	
3		water	18.020	1.0000
4		yeast		
5		Enter name here		

6. In the **Mixtures** tab, create any mixtures of chemicals that you plan to use. To do so, provide a name for your mixture, such as “1 mM NaCl”. Next, click and drag the chemical name from the map panel (upper left) to the mixture line you are creating. Add additional chemicals, and units and amounts for your mixture as needed. Once finished you should see the mixture name in the map panel.

An example of a complete mixture:

Mixture					Component			
	Color	Name	Density	Inventory	Name	Role	Concentration	Unit
1		yeast activation	Not determ Ideal Mixing		yeast		.0120	mg/ml
					water			remainder

7. In the **Parameters** tab, you will find the various options for controlling the operation of the robot. For example, the parameter “Uncap” tells the system to uncap a vial, and “StirRate” sets the stir rate for a plate. For any parameters you want to use, click and drag the parameter from the list in the lower left to the list in the lower right. You should now see the parameter in the map panel (upper left).


At the moment, all parameters require the use of the Processing tag (more on that later, we will remind you when it comes up). Some important ones are:

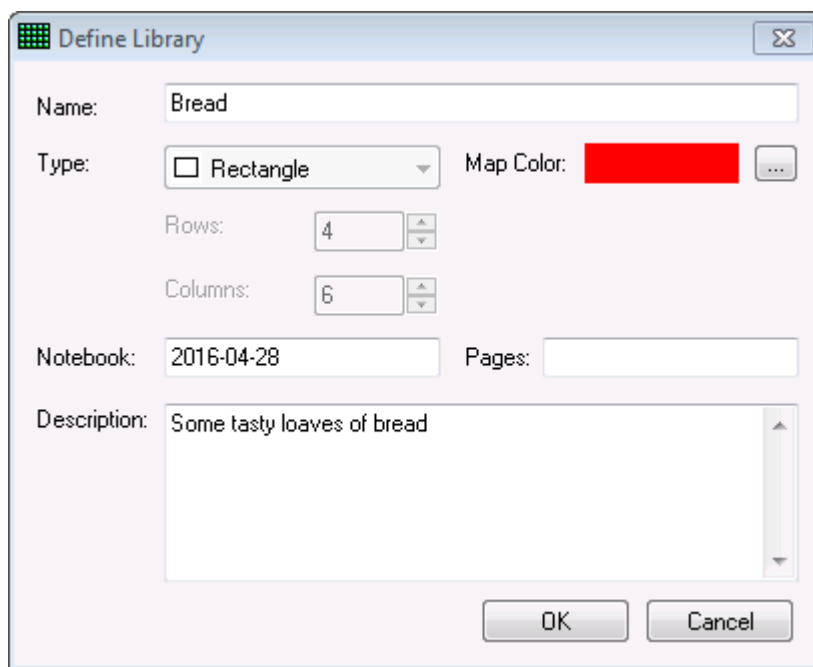
Parameter	Usage
Cap, Uncap	The given vial will be capped or uncapped when set to 1.
Tare, Weigh	Measures the mass of the vial when set to 1. If you use Tare, the weight is referenced when you use Weigh, and the difference between the two masses is recorded. By default, the masses of solids are recorded, but not the masses of liquids. If you want to weigh a dispensed liquid, you must specify use these tags to do so.
StirRate, VortexRate	Specifies the stir or vortex rate for the plate, in rpm. You will have to make sure the plate is in the correct position for this to work.
HeatingTemp	Specifies the heating temperature for the plate, in °C.
Delay	Tells the system to wait for some amount of time before proceeding. For example, if you need a hot plate to reach a temperature, use a delay to let it stabilize before proceeding.
SetTimer, WaitForTimer	If you want to let some operation happen but can perform other steps in the meantime, start a timer using SetTimer. Then, when you need that task to finish before proceeding, set WaitForTimer to 1.

8. Now that you have defined your chemicals and mixtures, and started to think about the operations the robot needs to perform, we will start to build the **Recipe**.
9. First, we will create a Library, which represents a physical plate on the robot deck. Currently, we have the following plates:

- 2x4 (20 mL or 40 mL vials)
- 4x6 (4 mL or 8 mL vials)
- 6x8 (2 mL vials)
- 8x12 (1 mL vials)

If the library you want to use already exists, you can skip the rest of this step.

To create a Library, click the icon , then provide the dimensions and useful name for this plate. For our example, we will create 24 loaves of bread:



The image shows a 'Define Library' dialog box. It has a title bar with a grid icon and the text 'Define Library'. The dialog contains the following fields and controls:

- Name:** A text box containing 'Bread'.
- Type:** A dropdown menu with 'Rectangle' selected.
- Map Color:** A color selection area showing a red square and a small '...' button.
- Rows:** A numeric input box with '4' and up/down arrow buttons.
- Columns:** A numeric input box with '6' and up/down arrow buttons.
- Notebook:** A text box containing '2016-04-28'.
- Pages:** An empty text box.
- Description:** A large text area containing 'Some tasty loaves of bread'.
- Buttons:** 'OK' and 'Cancel' buttons at the bottom right.

10. Once the library is created, we can start forming our recipe. In the map panel (the upper left), click on a chemical, then select the wells you want to add this to. You should see a menu like this:

**Define Map** ✕

To change cell selection, select new cells. To extend cell selection, Shift - Click or Ctrl - Click new cells.

Map Uniform ▾

Properties	Values
Source	sodium chl
Dispense Unit	mg
Design Unit	mg
Value	2

Tags: (none) Select...

☐ Amounts

Map Values



	1	2	3	4	5	6
A	2	2	2	2	2	2
B	2	2	2	2	2	2
C	2	2	2	2	2	2
D	2	2	2	2	2	2

OK Cancel

The “Design Unit” specifies the units for the amount you want to dispense, e.g. mg,  $\mu\text{L}$ , or mmol. The “Dispense Unit” is the method for dispensing this compound, either as a solid or liquid. These do not have to be the same, so long as you provide the density (dispensing liquid by mass) or molecular weight (dispensing reagent by mol) needed for unit conversion.

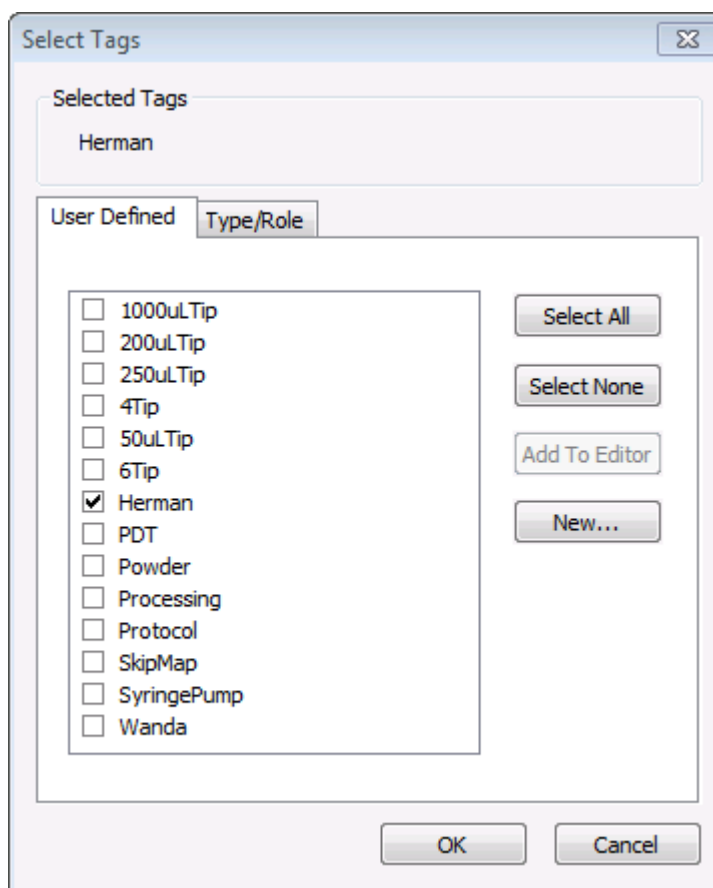
The “Map” options permit you to choose how much is added to each well. For our purposes we will be adding the same amount to each well, but we can also program gradients, individual amounts for each well, or other variations.

11. Once you have created your map, it should show up in the recipe list:

Maps	Tags
 Add 2 mg sodium chloride to Bread (A1:D6) in mg	none
 Add 500 ul water to Bread (A1:D6) in ul	none

12. The final step for creating a map is to specify Tags. Tags are the method by which we indicate what sort of step is being performed, and how it is to be done. For example, perhaps I want to Dispense my water using the 6-tip dispense tool, using 1000  $\mu\text{L}$  tips: for this, I would choose the “6Tip” and “1000uL” tags.

To add a Tag, right-click on a given map in your **Recipe** and select “Tag All...” (you can tag multiple maps at once). You should now see the list of available tags:





Check the box next to the tags you want to use. **Every map for HERMAN must have the “Herman” tag or it will not be recognized.**

Here are the tags and their usage:

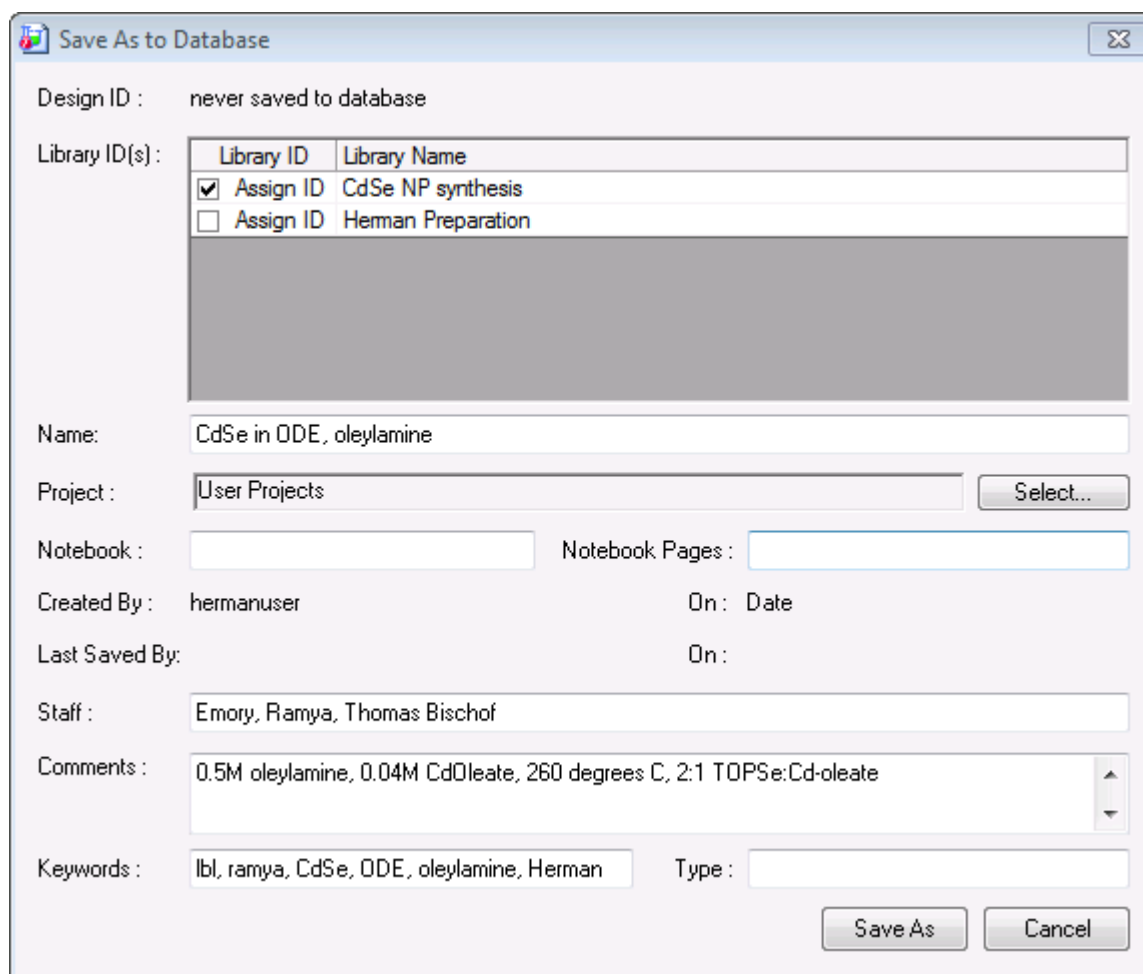
Tag	Applies to...	Usage
<b>Herman</b>	<b>All operations on HERMAN</b>	<b>Add this tag to anything that is to be run on HERMAN. Unless you are working with Wanda, all maps should have this tag.</b>
4Tip	Any liquid source	Specifies usage of the 4-tip tool for the dispense. This is only available for 8x12 plates due to the fixed pitch of the tips.
SyringePump	Any liquid source	Species usage of the extendable tip of the 4-tip tool. This is available for all plate dimensions.
6Tip	Any liquid source	Specifies usage of the 6-tip variable-pitch tool for the dispense. This is available for 4x6, 6x8, and 8x12 plates. Also specify the desired tip size using a “50uL”, “200uL”, or “1000uL” tag.
PDT	Any liquid source	Specifies usage of the single-tip PDT tool, typically for viscous liquids. Also specify the desired tip size using the “250uL” or “1000uL” tag.
Powder	Any solid source	Specifies that the given dispense is a powder.
SkipMap	Any map	Indicates that the map will not be run. This effectively is a comment, allowing you to leave a note indicating some future behavior during testing, or some step which involves manual intervention.

- Once you have created all of your maps, take a moment to check that the order, amounts, and tags all look correct. Are all maps tagged with “Herman”?

14. For some complex workflows, you might need to work with one or more library. To do so, simply create another library, and include it in your **Recipe**. If you want to move some content from one vial to another, you can use create a dispense map by clicking the icon for the source library in the map panel, selecting the wells to draw from, and then picking the wells to dispense into.
15. It is helpful to use the **Worksheet** tab to see how much of each source will be used. You will need somewhat more than this for your work, since containers cannot be completely emptied. You can also double-click a well to see its contents.

Source				
Color	Name	Min Amount	Amount To Make	Unit
	sodium chloride	48.000 mg	48.000 mg	
	water	12000.000 ul	12,000.000 ul	

16. At this point, you have a complete design which can be executed by the robot. Go ahead and save your design to the database by selecting **File/Save As.../To Database...**. You should see a menu which looks like this:



The dialog box titled "Save As to Database" contains the following fields and controls:

- Design ID :** never saved to database
- Library ID(s) :** A table with columns "Library ID" and "Library Name".
 

Library ID	Library Name
<input checked="" type="checkbox"/> Assign ID	CdSe NP synthesis
<input type="checkbox"/> Assign ID	Herman Preparation
- Name:** CdSe in ODE, oleylamine
- Project :** User Projects (with a "Select..." button)
- Notebook :** (empty text box)      **Notebook Pages :** (empty text box)
- Created By :** hermanuser      **On :** Date
- Last Saved By:**      **On :**
- Staff :** Emory, Ramya, Thomas Bischof
- Comments :** 0.5M oleylamine, 0.04M CdOleate, 260 degrees C, 2:1 TOPSe:Cd-oleate
- Keywords :** lbl, ramya, CdSe, ODE, oleylamine, Herman      **Type :** (empty text box)
- Buttons:** Save As, Cancel

Check the boxes next to "Assign ID" for all of your libraries, and fill out the remaining boxes as desired. Your "Project" should be "User Projects".

Once you choose "Save As", your libraries and design will be given ID numbers. Note these, as you will need to use them later when you run the robot or want to access your data.

## 2.2 Making a Design For HERMAN and WANDA

HERMAN is particularly well-suited for dosing reagents and performing parallel reactions, while WANDA is well-suited for running detailed serial reactions. As such, a common workflow is to prepare reactions in HERMAN, then transfer the vessels to WANDA for use.

Here we describe the specific steps and considerations for ensuring this process works smoothly. For an example of a successful design, see 1051 from the database.

1. First, read Section 2.1, and the manual for WANDA. You should have a good understanding of how to work with Library Studio before proceeding.
2. In Library Studio, open the template `prepare_in_herman_run_in_wanda.lsr`, which is in `My Documents ▸ library_templates`. This will serve as our starting point.
3. In this design, we have two libraries: one 8x1 library representing the 8 LTMR reactors in WANDA, and a 2x4 library representing a plate in HERMAN. Our general process is to perform dispense and other operations on the “Herman preparation” library, then physically move the vials to the “CdSe NP synthesis” library (you can rename these libraries as desired).
4. Build your `Recipe` for the “Herman preparation” library by following the steps outlined in Section 2.1.
5. In the `Recipe`, there are two maps noting the transfer of liquid from the “Herman preparation” library to the “CdSe NP synthesis” library. There is no way to automatically move the complete contents of a well, so you should instead determine the total contents of your wells (double-click on them in the library), and move that amount. This step is not strictly necessary but ensures that sensible values are shown in the `Worksheet` tab and the wells in the “CdSe NP synthesis” library. In the template, this volume is just over 9000  $\mu\text{L}$ .
6. Ensure that all maps which are to be performed by HERMAN are tagged “Herman.”
7. Ensure that the maps which transfer the contents of “Herman preparation” to “CdSe NP synthesis” have no tags. Since these are manual steps, we want to make sure that neither WANDA nor HERMAN will attempt to process them.
8. For the remainder of the maps for the “CdSe NP synthesis” library, follow the instructions found in the WANDA manual.

## 2.3 Loading Recipes From Spreadsheets

When designing your experiments, you may be accustomed to using Excel or another spreadsheet-style program for determining the quantities of various reagents to be used for each sample. In this Section, we will describe how to format your spreadsheets to enable you to import these data into Library Studio automatically, using the Design of Experiments (DOE) feature.

### 2.3.1 Building a Spreadsheet for Library Studio

The format that Library Studio expects is:

1. Each row represents a well in a library, filling horizontally (iterate through columns, then rows)
2. Each column represents the reagent to be added to that well.

Thus a valid file might look like the following:

Row	Column	flour	water
		mg	ul
1	1	10	500
1	2	10.5	500
...	...	...	500
8	12	20	500

Make sure that the row with your chemicals' names is consistent with your other work: these names will be used exactly as given, which is why the units are on a separate row. Once you have created a spreadsheet in this format, export it as a CSV file with comma delimiters.

In Library Studio, create a new design or open one which you wish to modify. Load your data using **File/Import/DOE Data**. Once you have chosen the file you should see a window like:

Design of Experiment Data Import - sample\_doe.csv

DOE - File Import

Header lines in import file(s)

Line number with factor names: 1

First line with data: 3

Edit Factor Names...

For later searching

Design Keyword (Optional)

Delimiters

Separated by: ☐ Tab ☐ Semicolon ☐ Other  ☒ Comma ☐ Space

Data Preview

	Row	Col	yeast	water	flour
1	1	1	10	500	0
2	1	2	10	500	45.454545
3	1	3	10	500	90.909091
4	1	4	10	500	136.36364
5	1	5	10	500	181.81818
6	1	6	10	500	227.27273
7	1	7	10	500	272.72727
8	1	8	10	500	318.18182

< Back Next > Cancel

Make sure the delimiter matches your CSV file. The “Line number with factor names” is the row where you have given the names of your chemicals. Change this and “First line with data” as needed to make your data appear sensible in the spreadsheet. Choose “Next>” when finished.

Now we must identify the chemicals:

	Factor	Source Type	Units	Map to	Additional
1	Row	[Ignore]			
2	Col	[Ignore]			
3	yeast	Chemical	mg	[Create New]	
4	water	Chemical	ul	[Create New]	
5	flour	Chemical	mg	[Create New]	

For each of the chemicals, we note the “Source Type” as “Chemical”, and provide units which match the ones we originally designed with. Finally, if the chemical already exists in Library Studio, select it under “Map to”, otherwise choose “[Create New]”. Choose “Next>” when finished.

Now we create the library:

DOE - Library Definition

Please confirm the new library dimensions and other properties:

Number of wells required: 96

Number of libraries to create: 1

Library Dimensions

Rows: 8

Columns: 12

Fill Direction

☒ Horizontal

☐ Vertical

Total Well Volume

☒ Constrain Total Volume to 0 ul

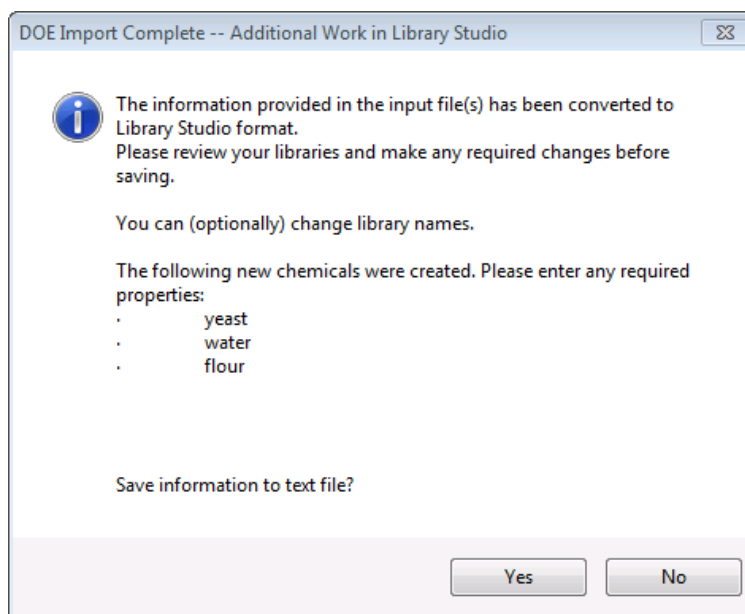
Fill Reagent:



Select the number of rows and columns in your design. Since we filled columns first, choose "Horizontal" for the "Fill Direction." Choose "Next>" when finished.

You should see a summary of the imported library. Choose "Finish" if this looks reasonable.

Finally, if you added any new chemicals you will see a dialog which looks something like this:



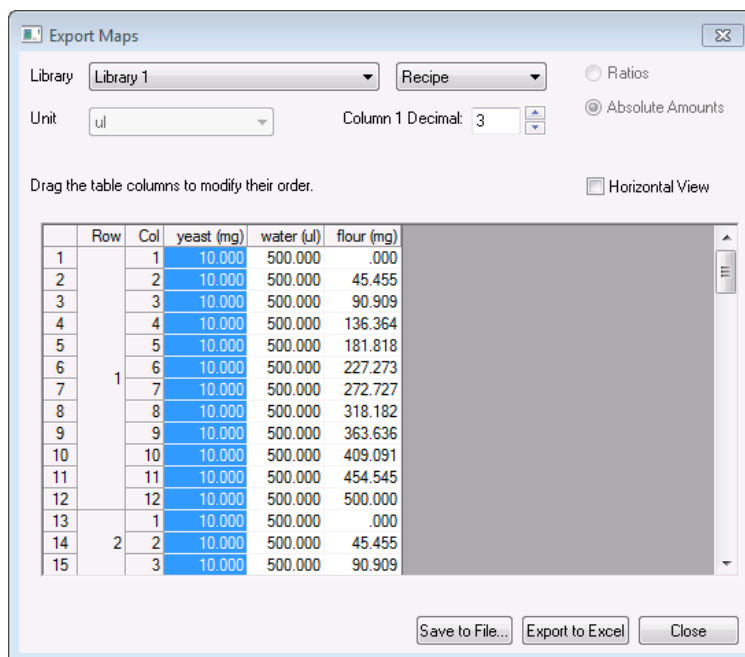
If you choose "Yes" the contents of the dialog will be saved to file. This can be useful as a sanity check: if you expected a chemical to already exist, make sure you did not accidentally create a second copy due to a typo.

At this point, you should now have maps in your Recipe (in the same order as the columns), and the chemicals in your inventory. You now can build the rest of your recipe by following the manual for HERMAN or WANDA, including tagging and other operations.

### 2.3.2 Advanced usage

#### Exporting designs to file

Build a Design or load one from the database. Select `File/Export/Maps...` to see this dialog:



Make sure to select “Recipe” from the list next to the library name. This ensures that all maps in your recipe are exported, including parameter maps.

Note that, during export, the chemicals will all be named with their dispense units. If you subsequently try to import this file, you will need to modify the chemical names to remove the units.

## Parameters

It is possible to specify parameters in your DOE files. This is done in the same way as specifying chemicals, except that you declare the “Factor” as a “Parameter.” You must provide information about the parameter, such as its data type, and this must match the definitions used elsewhere in Library Studio.

## 2.4 Pitfalls And Limitations

There are many tools and deck elements which can be used in many different configurations. Not all of these are physically possible, and the system is not always aware of these limitations, so it is up to you to make sure your design is valid.

Here are a few known limitations of the system, and how they will be handled.

### 2.4.1 Powder Dispense Using Both SV and Classic Hoppers

If your Design requires the dispense of solid compounds from both SV and Classic hoppers, you will be required to manually change the tools out. The “Sample Preparation” protocol is aware of this physical limitation and will warn you during startup that this is required, and will pause the protocol to wait for you to exchange the SV tool and Classic hopper when required.

### 2.4.2 The Deck Currently Supports Up to Three Disposable Tip Racks

There are currently four available tip box positions, one of which is used as a trash bin for PDT tips. If your design requires the use of four or more different types of tips, it will not be able to run properly.

### 2.4.3 Moving Plates Is Possible Not Advised

The protocol has no checks to ensure that plates movements are valid, that is, that the deck positions specified are not occupied. If you want to use this feature, contact Thomas or Emory to learn how to do so, and to make sure your design will work properly.

### 2.4.4 If You Use Capping, All Vials Must Start in the Same State

Currently, there is no way to specify that certain vials start capped or uncapped, merely that they are all capped, or all uncapped. All libraries which has some capping or uncapping performed must start in the same states (all capped, or all uncapped).

### 2.4.5 There Are No Automatic Checks to Ensure Your Layout Is Sensible

Library Studio permits you to do roughly anything you desire, regardless of whether it is physically possible to perform on the robot. It is your responsibility to ensure your design will operate properly, by understanding the limitations of the system and working with an expert to validate your options.



## Chapter 3

# Setting Up the Robot Deck

So, you now have a Design prepared, and want to get started actually running it. Before you can do this, you will need to set up the various deck elements, reagents, vials, and tools needed to process your design. In this Chapter, we will guide you through this process.

1. First, we must determine what plates, tools, and deck elements you will need.
  - (a) Open your Design in Library Studio, and note which plates you will need (one per Library). Obtain these plates and set them in the bays on Deck 10–11 (and 12–13, 14–15, as necessary).
  - (b) If you cannot fit all of these plates on the deck, stop and reflect: do you really need these many plates? If so, consult Thomas or Emory to find a solution.
  - (c) Next, read through your list of [Chemicals](#) and [Mixtures](#), and check the amount of each you need in the [Worksheet](#). How many distinct sources do you use, and what size containers are appropriate for storing them?
    - i. For solids, you have two options: 4 mL SV hoppers, or a 25 mL Classic hopper. Lay out empty hoppers in their positions on Deck 1–2, until you have enough to hold all of the solids you plan to dispense.
    - ii. For liquids, you have several options: various vials, 30 mL 8x1 reservoirs, 250 mL reservoirs, or backing solvent (xylene). Lay out empty vessels for all of the liquids you plan to dispense.
      - A. Are your liquids volatile? Workflows can take quite some time to complete, and so things like methanol have a tendency to evaporate before you can use them. For these liquids, try to use containers with small openings, and have plenty extra on deck.
    - iii. Read through your [Recipe](#) and note the methods for dispensing liquids.
      - A. For the “4Tip” and “SyringePump” tags, nothing is required.
      - B. For the “6Tip” and “PDT” tags, what size tips do you plan to use? How many tips are going to be needed? Put these tips in Deck 8–9. **Make sure the ADT tip boxes are orientated such that the “Front” label is in front**
  - (d) At this point, you should have:
    - Plates with vials for each library in your design.
    - Hoppers ready to be filled with your solids.
    - Reservoirs ready to be filled with your liquids.
    - Pipette tips ready to be used.
2. For all of the solid dispense hoppers and liquid reservoirs, add enough material to cover the amount you plan to use, plus about 30 % extra.



3. Now, open Automation Studio .

4. In Automation Studio, open the Chemical Manager (Tools/View Chemicals...). For each chemical and mixture you plan to use, fill out the following information:
  - (a) Name: The name of your chemical, as shown in your design in Library Studio. **This must be the exact name used in the design.**
  - (b) Container Size/Actual Amount/Units: You can keep track of the amount of each source which is left by filling these out. If you have two or more vials for storing these materials, the system will automatically switch between them as one empties. If none are available, the instrument will halt and prompt you for more, instead of continuing as though nothing is wrong.
  - (c) Off-deck: If you are dispensing backing solvent (xylene): check this box, choose "Syringe 7" as the Valve Resource, and set "1" as the Valve Position. Otherwise do not check this box.
  - (d) Substrate: This is the type of vial or reservoir you are dispensing from. Typically, you will want to pick from:
    - Rack 3x4 SV Hopper
    - Rack 1x1 25 mL Hopper (Classic Hopper)
    - Rack 2x4 20mL Vial (typically for PDT)
    - Plate 8x1 Reservoir (typically for 6-tip or 4-tip)
    - Plate 1x1 Reservoir (for any liquid dispense)
  - (e) Position: The location on the deck (e.g. Deck 10–11)
  - (f) Row, Column: The position on the substrate for your particular reservoir. Note that these are numeric, so "A1" becomes Row 1 Column 1.
  - (g) Dispense Category:
    - For solids: use "Powder Accuracy"
    - For liquids: if you are using a PDT, "PDT Dispense." Otherwise, "Non-Viscous Liquid"
  - (h) Dispense Mode:
    - For solids: "Powder Setting"
    - For liquids: select "PDT" if using the PDT tool, and "ADT" otherwise.
5. In the Chemical Manager, click "Save".
6. If you are using the SV Hoppers or the Classic Hopper, which is used first? If the SV Hoppers are used first, place the SV tool in Deck 1–2. If the Classic Hopper is used first, place it in Deck 1–2.
7. At this point, you should have:
  - Plates with vials for your libraries
  - Reservoirs with your starting materials
  - Tips and tools for performing dispenses
  - Trash bins for your disposable tips.

Take a moment to check that nothing has been left out.

8. (optional) Take a photograph, or write down this configuration for your notes. If you need to run a similar experiment, having this layout in your mind will greatly simplify the process of setting things up next time.

You can also export the information in Chemical Manager (Tools/View Chemicals..) by choosing "Export".

9. If everything is okay, you are ready to start running your experiment.


## Chapter 4

# Running the “Sample Preparation” Protocol

### 4.1 Checklist For Starting Up

1. **Sign up for time on the online calendar.**
2. Check the levels of the backing solvent.
3. Open the solvent trap (use gloves to handle the switch) and make sure it is not full.
4. Check that the waste bins on the deck are not full.
5. Make sure the robot is on: the green “Start” button behind the monitor should be lit. If it is not:
  - Try pressing the “Start” button. If it lights up, you are done.
  - If that did not work, check that the main power switch is on. This is located on the grey box on the bottom of the glovebox, underneath the computer monitor. If this was off, turn it on and try pressing the “Start” button.
  - If that did not work, check that the red “Stop” buttons (two on front, one in the rear) are activated by rotating them clockwise.
  - If none of these steps worked, find someone knowledgeable to troubleshoot the issue.



6. Open Automation Studio . Near the top, make sure the box says “Hardware Enabled.” If it says “Hardware Disabled”, click on it once to enable the hardware.
7. **Sign the log book.**

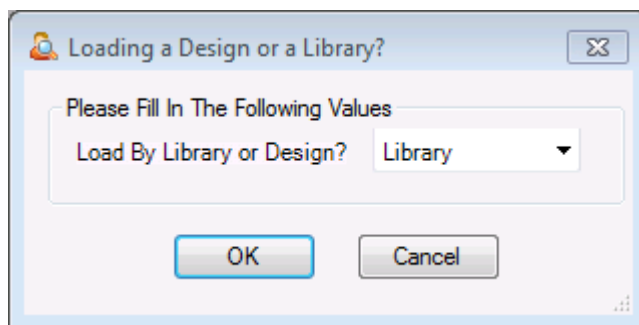
### 4.2 Checklist For Shutting Down

1. Remove your compounds and samples from the deck.
2. Clean the deck elements by wiping down with toluene, then isopropanol.
3. Close the solvent trap (use gloves to handle the switch)
4. Check that the time you signed up for in the online calendar is accurate. Update it if necessary.
5. **Sign the log book. Note any errors or issues, and tell Thomas or Emory what went wrong.**

## 4.3 Running “Sample Preparation”

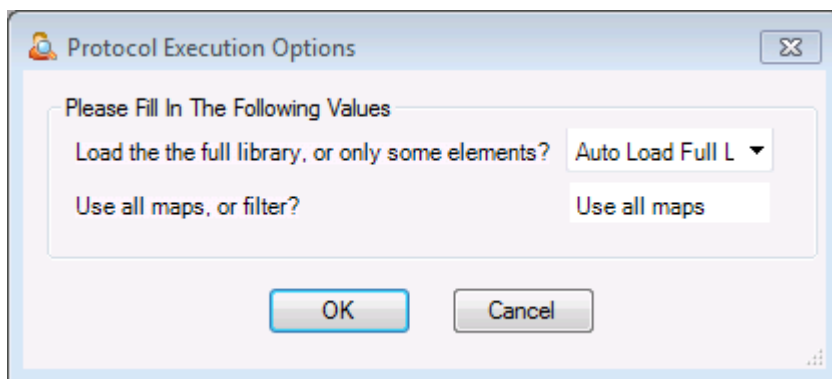
In this Section we describe how to run an experiment. You are expected to have already created your design (Chapter 2) and set up the deck with your materials (Chapter 3). Make sure to do so before proceeding.

1. At this point, Automation Studio should be open, and the CM3 System UI should be visible. If the UI is not visible, open it with `Hardware/CM3 System UI`
2. In the UI, click the “Sample Preparation v2” button. This will require about 30s to load completely.
3. You should now see the following menu:



Typically, you will want to load a Library. If your design is only used for HERMAN, you can load by design. **If your design involves WANDA at all, only load by Library.**

4. Next, you should see:

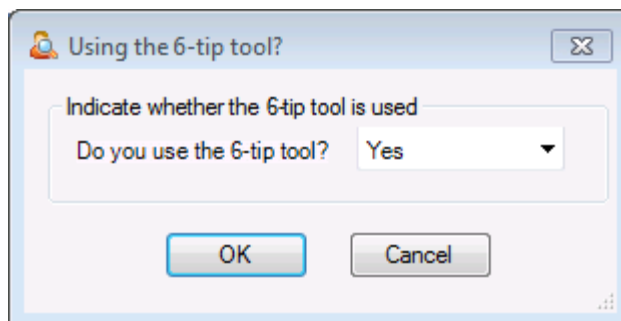


Most of the time, you should load the full library: empty wells will be ignored. If you only want to run certain wells, choose “Load Selected Elements”, which will later prompt you for the exact wells to run.

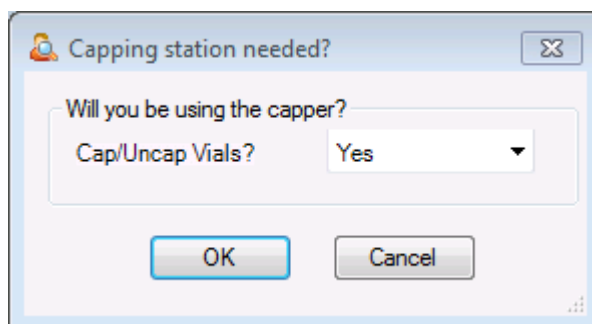
As for the second line, typically you will want to run your whole recipe. Sometimes though, you might want to only run maps with particular tags (in which case say “Only certain Tags”), or perhaps just specific maps (in which case, “Choose specific maps”). If you pick either of these options, you will be prompted later.

5. Are you using the 6-tip tool in your library?

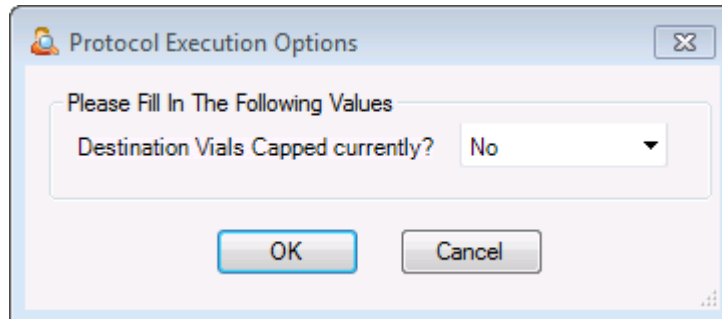




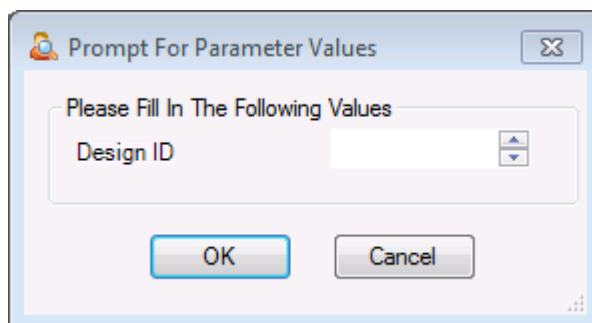
6. Are you going to cap or uncap vials?



If you do use the capper, are the vials currently capped? Note that all vials which are to be capped or uncapped need to be in the same state (all capped, or all uncapped).

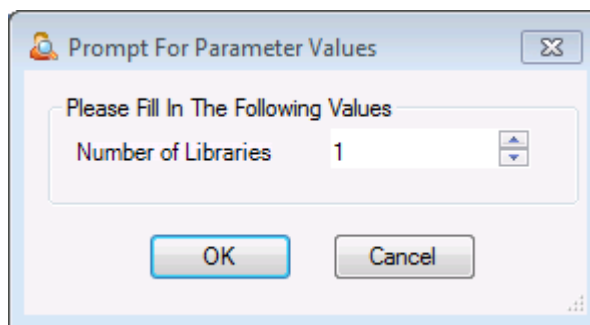


7. If you are loading by Design, provide the Design ID (4-digit number). This can be found in Library Studio in the title bar at LBNL-xxxx.

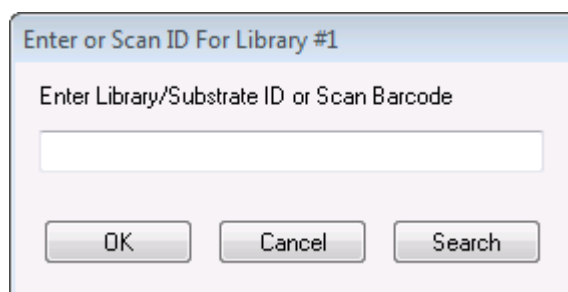


Note that loading by Design changes the order of options slightly: you will be shown the maps to be executed before selecting substrate locations. This is normal, if a bit confusing.

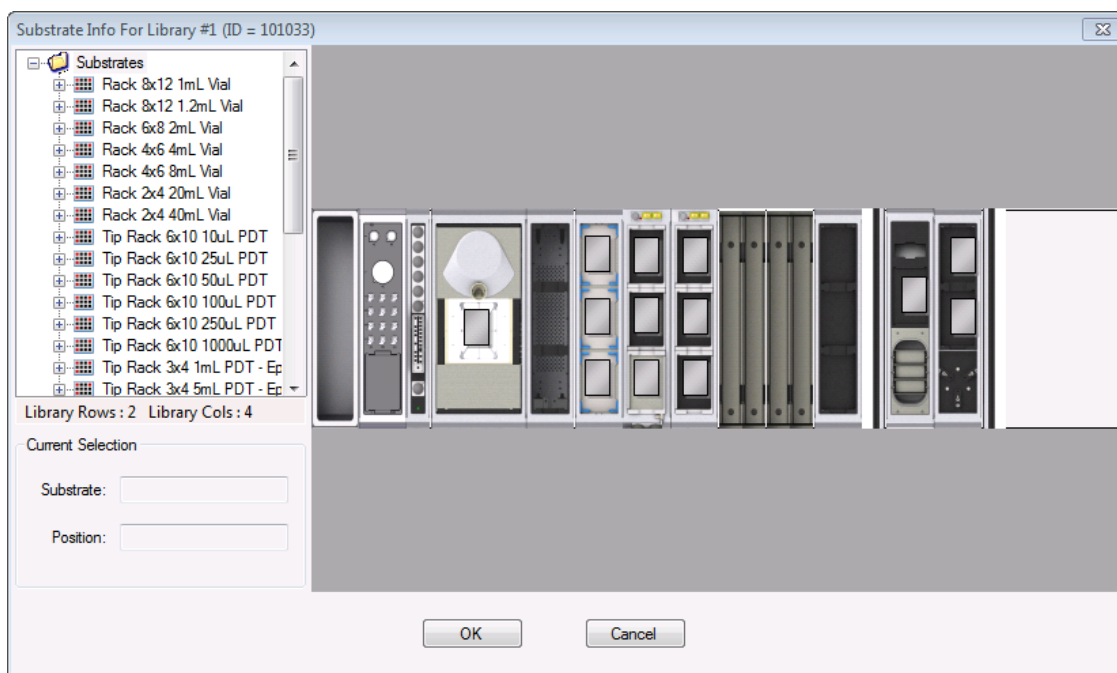
8. If you are loading by Library, you can load more than one at once:



Provide the ID (6-digit number) for each library. This can be found in Library Studio on the plate as LBNL-xxxxxx.



9. As you start loading designs and libraries, you will be asked for their physical location on the robot deck:



Start by choosing the type of plate associated with this library (e.g. Rack 2x4 20mL Vial), by clicking on the name in the left-hand panel. Then either select the deck position from the picture or the expanded list.

Take a moment to look at the deck: does the type of plate match what you have chosen? Is it in the right place?

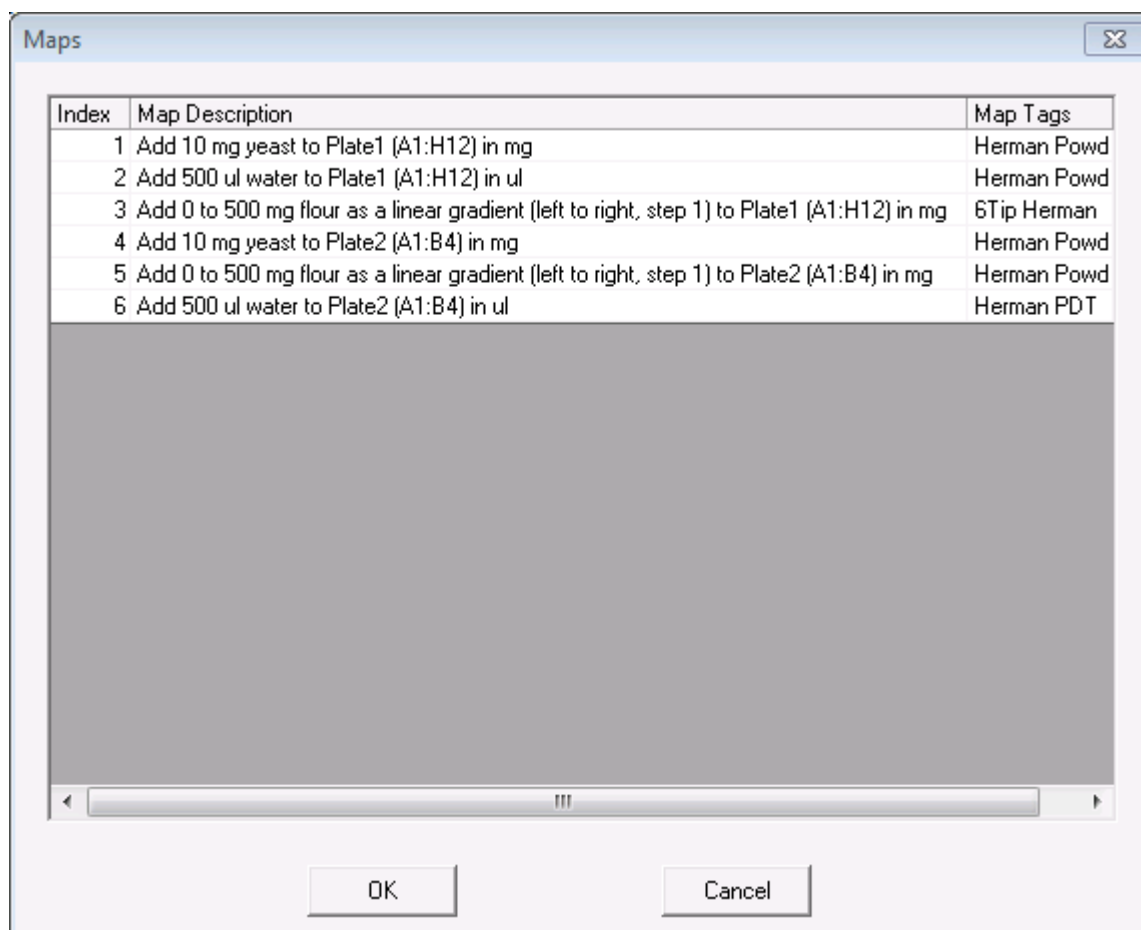
10. Select the locations and substrate (plate) types for all of your libraries.

11. Now you are prompted for all chemicals used in your experiment:

	Name	Percent Amount	Actual Amount	Container Size	Units	Off-Deck	Substrate	Position	Row	Col	Valve Resource	Valve Position
	flour				mg	<input type="checkbox"/>	Rack 3x4 SV Hopper	Deck 1-2 Position :	1	1		

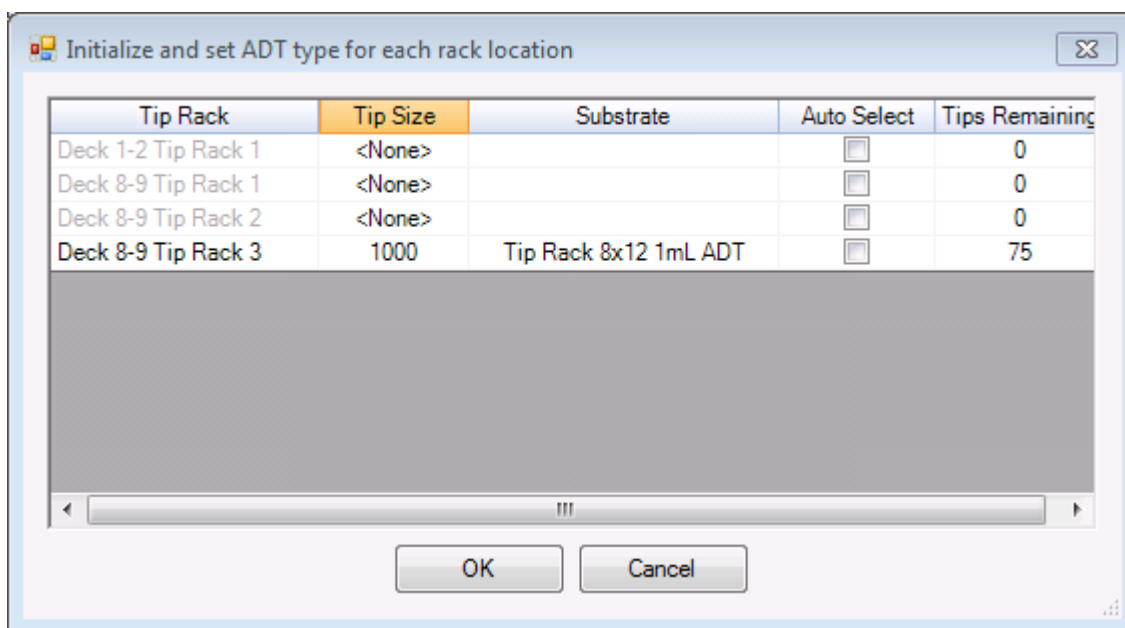
Follow the instructions in Chapter 3 if this list is incomplete. Take a moment to check each entry: does it match what you expected? Are the locations and amounts of sources accurate? Are the dispense methods correct? If anything is incorrect, change it now.

12. At this point, you have specified all of the options for running your experiment. You should now see a list of all of the maps which are to be executed:



If this looks right, press OK. If not, what is wrong? Did you mean to filter the maps? Are you maps tagged appropriately? Are your maps tagged “Herman”? **If this does not look right, press Cancel.**

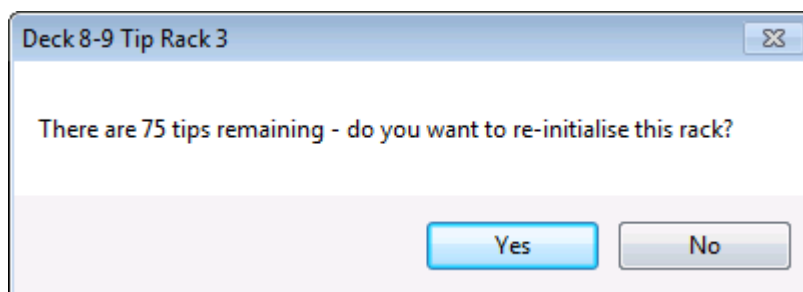
13. If you are using ADT or PDT disposable tips, you will be prompted for the locations of these boxes:



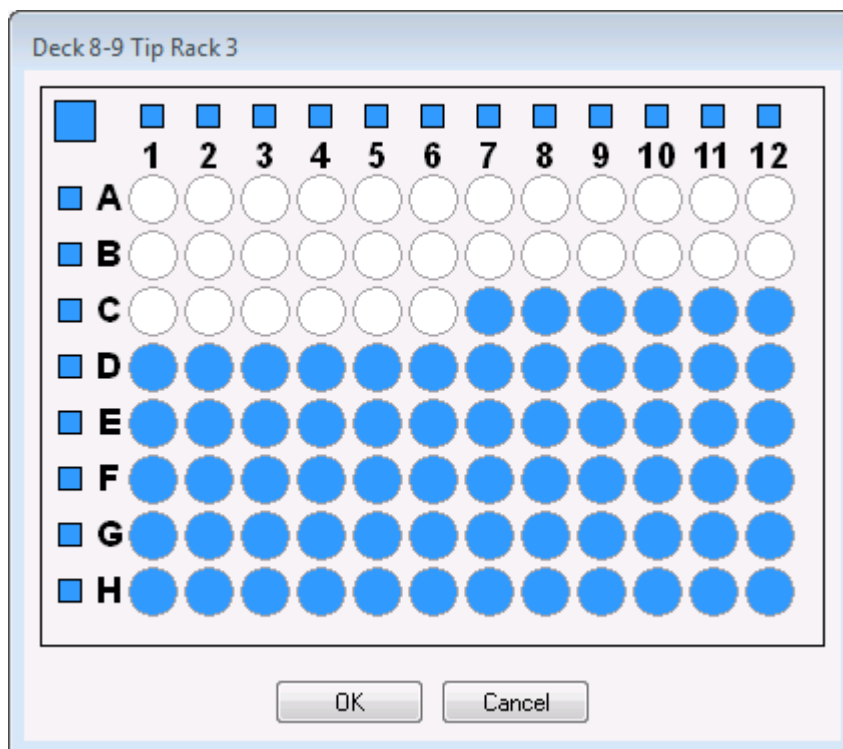
Make sure that the boxes you have on the deck are reflected here, that the location and tip sizes are accurate. Do not use “Auto Select” unless the box is completely full. The valid tip sizes are:

- (a) ADT: 50  $\mu$ L, 200  $\mu$ L, 1000  $\mu$ L
- (b) PDT: 250  $\mu$ L, 1000  $\mu$ L

For each tip rack, you will ask asked whether it should be initialized:

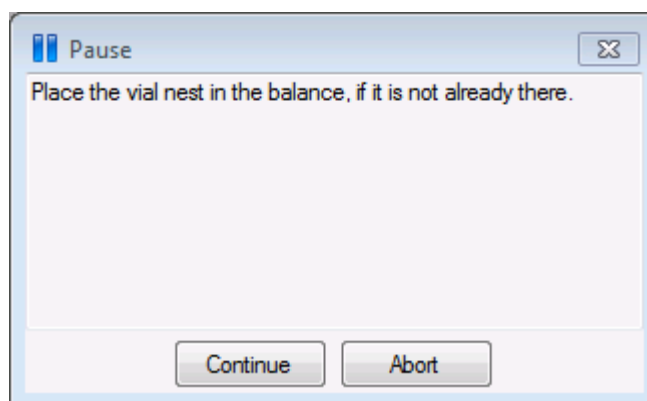


Click Yes to initialize the tips.

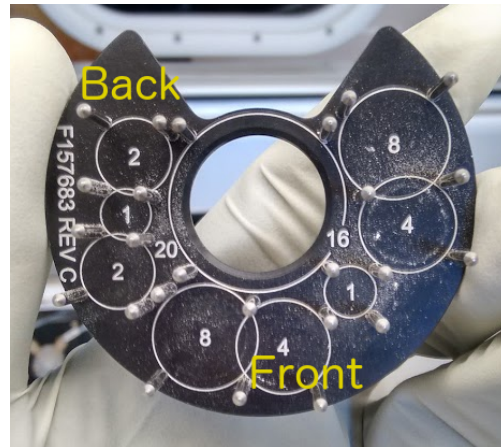


Click on wells (or rows/columns) until the image matches the tips in the box (blue means a tip, white means no tip). **For ADT tips, only fill in complete sets of 6 tips, starting from the end. Even if you have a row partially filled with tips, do not include these.**

14. If you are using the balance, the system will determine whether or not you need the vial nest. **If your design requires the use of the balance for various sizes of vials, you will see a dialog indicating that you must manually move the nest at various times. If you do not follow these prompts, your experiment will not run to completion.**
15. When prompted, move the vial nest into or out of the balance:



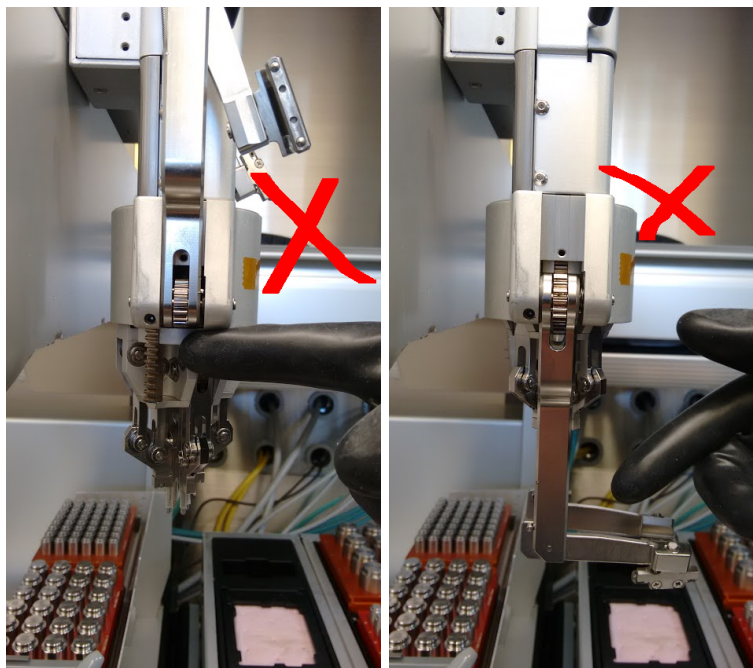
Note that the vial nest should be oriented properly in the balance, such that it is centered and the front faces forward:



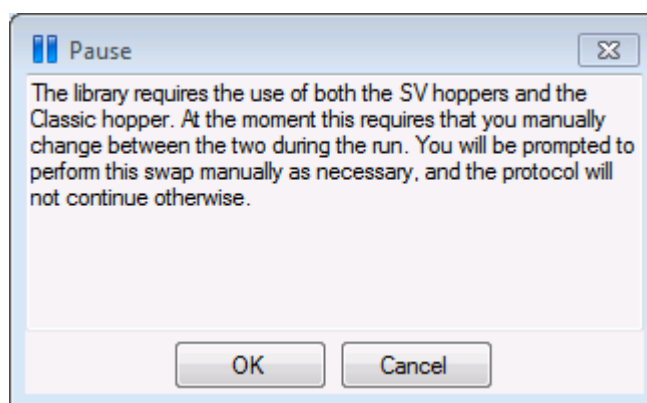
16. You are now prompted to fold up the plate gripper (right-hand side of the right arm). It should look like this:



Not like this:



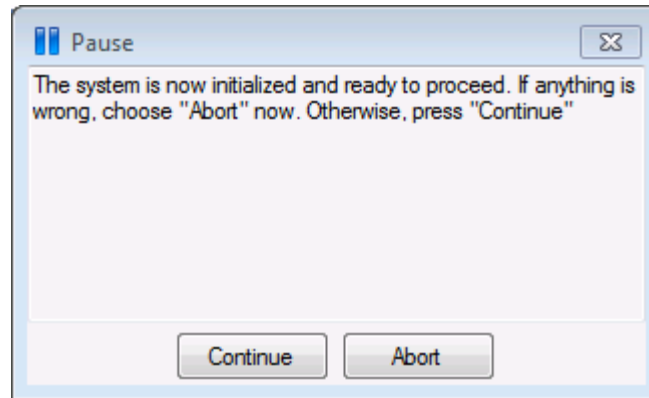
17. If you need to use both the SV and Classic hoppers, the system will now inform you that changing these tools is requires manual intervention. **If you see this menu, you will need to manually change the tools as required. If you do not do this, your experiment will not run to completion.**



18. If you use solid dispense, you will be prompted to set up the deck with the SV tool or the Classic hopper. Make sure these lie flat on the deck, and for the SV tool make sure the pin lines up with the slot on the deck.

19. At this point, you are done setting up the experiment.





This is a good time to have someone check to see if everything looks reasonable. **If anything seems wrong, now is the time to press Abort and start over.**

Press Continue if you want the experiment to run.

20. While running, you may encounter errors like “Specified Substrate Does Not Exist”. Talk to an expert to fix these problems.

If you understand what the error is, what causes it, and how to fix it, you can try troubleshooting. Some tips are provided in Appendix A.

21. If the robot runs into issues during the experiment (a vial drops, etc.) and the problem is minor, you can stop the system by activating the light curtain (put your arm in a glove, just past the glass). Have an expert help you diagnose the problem and help you restart the experiment.

**If the problem is major, press the red “Stop” button to halt the system and find an expert to help you fix things.**



## Appendix A

# Troubleshooting

### A.1 The stop button in the software may not stop the whole protocol

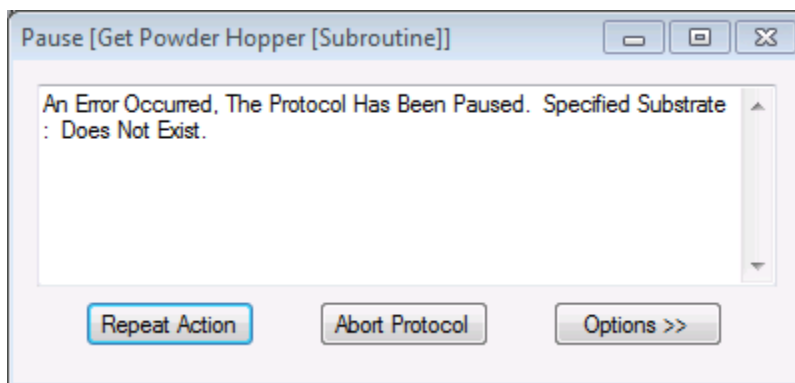
Sometimes, you might hit the stop button in the software, only to find that the robot moves on to some other step instead of completely halting. This is a quirk of the design: the software button halts the current sub-protocol but not the main one, so it might take three or more stops to actually halt the process.

**If you need to halt the system immediately, use the large red stop hardware button on the front or back of the machine.** Once you stop this way, you will need to kill the ASCore service and restart Automation Studio.

### A.2 One of my vials failed, how do I fix this?

If one of the your samples fails in some way (e.g. overdispense of a reagent), it is sometimes possible to rerun just that sample and keep the data consistent. Talk with an expert to learn how to do this.

### A.3 I got an error message, what does it mean?





## Appendix B

# Complete Listing of Map Tags and Parameters

Here we document all known parameters and tags used in either Herman or Wanda. This is meant to be exhaustive and as such contains much more information than you need. For an overview-level description of these options, see Chapter 2.

### B.1 Map Tags

#### B.1.1 50uLTip, 200uLTip, 250uLTip, 1000uLTip

##### Usage (Herman)

When used with either the PDT or 6Tip tag, this tag specifies the size of tip to use. If no tip size is specified, the smallest acceptable tip size will be used. Note that the ADT and PDT tips are not available in all of these sizes, so make sure that the size you choose is an option.

##### Sources and Parameters Affected

Any liquid source.

#### B.1.2 4Tip

##### Usage (Herman)

Specifies that the given liquid dispense map is to be performed using the 4-tip fixed tip tool.

##### Sources and Parameters Affected

Any liquid source.

#### B.1.3 6Tip

##### Usage (Herman)

Specifies that the given source is to be dispensed using the 6-tip disposable-tip tool.

##### Sources and Parameters Affected

Any liquid source.

### **B.1.4 Aliquot**

#### **Usage (Wanda)**

Aliquot times. Must be placed in chronological order.

#### **Sources and Parameters Affected**

Aliquot Time

### **B.1.5 Analysis**

#### **Usage (Herman)**

Unknown, found in “Sample Preparation”

#### **Sources and Parameters Affected**

Unknown

### **B.1.6 BottomDispense**

#### **Usage (Herman)**

Unknown, found in “Sample Preparation”.

#### **Sources and Parameters Affected**

Unknown

### **B.1.7 Cleaning**

#### **Usage (Wanda)**

Used by protocol “Cleaning Protocol ECx”. Cleaning steps will be performed in the order they are placed in the library.

#### **Sources and Parameters Affected**

Centrifuge, Supernatant, Vortex

### **B.1.8 DispenseTip**

#### **Usage (Wanda)**

Specifies that the left dispense needle tip is to be used for the given liquid source.

#### **Sources and Parameters Affected**

Any liquid source.

### **B.1.9 EmptyFootprint**

#### **Usage (Herman)**

If this tag is used, the line will not be executed. This is not the desired method for not executing a map (that is “SkipMap”), but this filtering is used at various points in the protocol.

**Sources and Parameters Affected**

Any map

**B.1.10 Gravimetric****Usage (Herman)**

Specifies that the given liquid dispense is to be performed with gravimetric feedback. (behavior not verified)

**Sources and Parameters Affected**

Any liquid source.

**B.1.11 HeatedTip****Usage (Wanda)**

Specifies that the right heated needle is to be used for the given liquid source. This is typical for molten surfactants.

**Sources and Parameters Affected**

Any liquid source.

**B.1.12 Herman****Usage (Herman)**

This tag is required for any map which is to be executed in Herman. If a map lacks this tag, it will not run.

**Sources and Parameters Affected**

Any map which is to be executed in Herman.

**B.1.13 Hover****Usage (Herman)**

For a given liquid dispense map using a single-output tool, move the vial to the capping station, uncap it while keeping the cap in the vial gripper, add the liquid, then recap the vial and return it to the original plate.

**Sources and Parameters Affected**

Any liquid dispense map.

**B.1.14 Initiate****Usage (Wanda)**

Identifies the source that is injected into the reactor to initiate the reaction (Workflow Step #3). If you do not use this tag, NOTHING will be injected at the "Inject Initiator" step (#3) of the workflow. If you have multiple sources tagged with the Initiate tag, then all sources will be injected sequentially, in their order in the recipe. The reaction time clock will be referenced to the injection of the last source.

**Sources and Parameters Affected**

Any liquid source to inject to initiate a reaction.

### **B.1.15 Interval**

#### **Usage (Wanda)**

Determines the times at which an aliquot will be collected. A map must also have the “Reaction” tag for an aliquot step to be completed.

#### **Sources and Parameters Affected**

Aliquot

### **B.1.16 LookAhead**

#### **Usage (Herman)**

Specifies that the liquid source is to be dispensed using a lookahead method. In this method, if the dispense volume is less than half of the tip capacity, multiple dispense volumes can be taken up into the tip in a single aspiration step, then dispensed piecemeal. This typically is used by the PDT, but can also be used by the ADT if accuracy is not critical (note: it is not verified that ADT dispense has this option implemented)

#### **Sources and Parameters Affected**

Any liquid source dispensed with a disposable tip.

### **B.1.17 Manual**

#### **Usage (Herman)**

If added to a dispense map, indicates that a given step involves manual intervention with the operation of system. This is typically used for a step involving a non-automatable task, such as the movement of a heavy object or the reconfiguration of the deck.

#### **Sources and Parameters Affected**

Any dispense map.

### **B.1.18 MoveVial**

#### **Usage (Herman)**

Unknown behavior. If used with 4Tip, the dispense will not proceed.

#### **Sources and Parameters Affected**

Any dispense map.

### **B.1.19 NewTip**

#### **Usage (Herman)**

(behavior is not yet verified) For a liquid dispense involving a disposable tip, this option discards the tips after each aspirate-dispense step.

#### **Sources and Parameters Affected**

Any liquid source dispensed with a disposable tip.



### B.1.20 OffDeck, OnDeck

#### Usage (Wanda)

Specifies whether the source is on the deck (in a vial rack) or off deck (backing solvent). By default, the protocol will look for the first available source in the Chemical Manager, starting from the top.

#### Sources and Parameters Affected

Any liquid source.

### B.1.21 PDT

#### Usage (Herman)

Specifies that the given source is to be dispensed using the PDT tool. To use a specific tip also provide a tag for the desired tip size, otherwise the smallest acceptable tip will be used. To change tips between dispense steps add the "NewTip" tag.

#### Sources and Parameters Affected

Any liquid source.

### B.1.22 Plate

#### Usage (Herman)

Specifies that the given dispense is to be performed on the balance to the whole plate, rather than in a standard deck position. This permits more rapid feedback of the mass dispensed, since the vials do not need to be moved, and enables dispense to a fixed substrate (e.g. an analysis plate). However, the extra mass of the plate reduces the accuracy of the weight measured.

#### Sources and Parameters Affected

Any dispense map

### B.1.23 Powder

#### Usage (Herman)

Specifies that the given source is dispensed as a powder. The first available source in the Chemical Manager determines the method used for dispense (SV or Classic).

#### Sources and Parameters Affected

Any solid source.

### B.1.24 Precipitant

#### Usage (Wanda)

Unknown behavior. Found in Design 750

#### Sources and Parameters Affected

Unknown

### B.1.25 PrepStir, PrepTemp

#### Usage (Wanda)

These tags are used to label deck temperature and stir parameters that should be set prior to the addition of the reagents (e.g. if reagents need to be heated and stirred to maintain solubility)

#### Sources and Parameters Affected

Heat-Cool-Stir Bay Temperature, Heat-Cool-Stir Bay Tumble Rate, Heat-Stir Bay Stir Rate, Heat-Stir Bay Temperature, LTMR Stir Rate

### B.1.26 Processing

#### Usage (Herman)

Specifies that a given map affects a deck parameter associated with plate movements, vial capping, or related tasks. Without this tag, such tasks will not be performed.

#### Sources and Parameters Affected

Cap, CentrifugeSpeed, CentrifugeTime, Delay, HeatingTemp, HoldCover, Pause, PlaceCover, PlaceHeld-Cover, RemoveCover, RunCentrifuge, SetTimer, StartTemperature, StirRate, Tare, Uncap, VortexRate, WaitForTimer, Weigh

### B.1.27 Protocol

#### Usage (Wanda)

Specifies that the given parameter is associated with a particular protocol name or version.

#### Sources and Parameters Affected

UseWithProtocolName, UseWithProtocolVersion

### B.1.28 Quench

#### Usage (Wanda)

Specifies the source to be added once the reaction has been quenched.

#### Sources and Parameters Affected

Any liquid source.

### B.1.29 Reactant

#### Usage (Wanda)

Required for any liquid chemical source that you want to add to a reaction vessel using the robot before a reaction.

#### Sources and Parameters Affected

For use by the “Add Components to Reaction Vials” protocol (TBA).

### B.1.30 Reaction

#### Usage (Wanda)

Required for any deck condition during the reaction such as temperature, stir rate, and dispense rate.

#### Sources and Parameters Affected

Aliquot Volume (uL), Dispense Rate, Growth Temperature, Heat-Cool-Stir Bay Temperature, Heat-Cool-Stir Bay Tumble Rate, Heat-Stir Bay Stir Rate, Heat-Stir Bay Temperature, LTMR Stir Rate, Nucleation Temperature, Quench Temperature, Reaction Time, Temperature Ramp Rate, Temperature Stability Delay

### B.1.31 Reactor

#### Usage (Herman)

Reserved for use with the custom reactor to be installed in Herman. This tag specifies that the given parameter is associated with the reactor. This will probably be merged with “Processing” once the reactor is installed, with the parameter implicitly assigned based on the location of the plate.

#### Sources and Parameters Affected

ApplyVacuum, PurgeReactor, HeatingTemp

### B.1.32 SafeWash

#### Usage (Wanda)

For washing reactive chemicals. After dispensing, the syringe tip will wash itself in dedicated on-deck containers before washing itself in the normal wash stations. In the Chemical Manager in Automation Studio, the user must specify the locations for the sources “SafeWaste,” “SafeWash,” and “SafeRinse”. In the SafeWash routine, the excess reagent will be dispensed in the SafeWaste, along with some backing solvent. The outside of the needle will then be rinsed in the SafeWash, and then the syringe will aspirate a set volume of the SafeRinse reagent and dispense it in the SafeWaste. Approximately 4 mL of waste is generated per SafeWash cycle.

#### Sources and Parameters Affected

Any liquid source.

### B.1.33 SkipMap

#### Usage (Herman)

If a map is given this tag, it will not be executed. This behavior is equivalent to having no tags, but enables the map to contain other tags for debugging or descriptive purposes.

#### Sources and Parameters Affected

Any map.

### B.1.34 Solvent

#### Usage (Wanda)

Used by protocol “Aliquot Plate Preparation ECx”.

---

**Sources and Parameters Affected**

The chemical source used for aliquot dilution

**B.1.35 SourceUncap****Usage (Herman)**

Given capped vials, this tag specifies that the vial should be uncapped, the dispense performed, then re-capped. This contrasts the whole-plate behavior typically implemented with “Cap” and “Uncap,” and minimizes the amount of time the vials remain open.

**Sources and Parameters Affected**

Any dispense map.

**B.1.36 SyringePump****Usage (Herman)**

Specifies that the given liquid dispense is to be performed using the

**Sources and Parameters Affected**

Any liquid map

**B.1.37 SyringeVolume1mL, SyringeVolume5mL****Usage (Wanda)**

Specifies which volume of syringe to use for dispense. When a source is tagged “Initiate”, the default is the 5 mL. Otherwise, the default is the smallest syringe which can handle the specified volume.

**Sources and Parameters Affected**

Sources tagged Initiate, and all other sources.

**B.1.38 Wait****Usage (Herman)**

When setting a temperature for one of the Heat-Stir-Cool or Heat-Stir bays, wait until the system has reached the specified setpoint before proceeding.

**Sources and Parameters Affected**

HeatingTemp

**B.1.39 Wanda****Usage (Wanda)**

A cosmetic tag indicating that the map is expected to occur in Wanda. Note that the actual behavior will be determined by the remaining tags; this tag does not affect the operation of the system in any way.

**Sources and Parameters Affected**

Any map.

### **B.1.40 Weigh**

#### **Usage (Wanda)**

After the addition of a source tagged “Weigh,” the robot will move the vials to the balance to record the actual masses of the liquids dispensed.

#### **Sources and Parameters Affected**

Any liquid source.

## **B.2 Map Parameters**

### **B.2.1 Cap/Uncap**

#### **Usage (Herman)**

When set to “1”, the specified vial will be capped/uncapped using the cap in the equivalent position on the cap rack.

#### **Associated Tags**

Processing (required)

### **B.2.2 Delay**

#### **Usage (Herman)**

Sets a blocking timer for the given amount of time. The system will do nothing until the timer finishes.

#### **Associated Tags**

Processing (required)

### **B.2.3 HeatingTemp**

#### **Usage (Herman)**

Sets the temperature for the given library. This assumes the plate is in a sensible position: there is currently no error-checking to ensure the plate actually can be heated in its present location.

#### **Associated Tags**

Processing (required)

### **B.2.4 SetTimer**

#### **Usage (Herman)**

Starts a non-blocking timer for the given amount of time. Because it is non-blocking the system will continue to execute other maps, until the “WaitForTimer” parameter is used. If the timer runs out the system will continue.

Currently, each library can have only a single associated timer. A new call to “SetTimer” overrides any existing ones.

#### **Associated Tags**

Processing (required)

### B.2.5 StirRate

#### Usage (Herman)

Sets the stir rate at the deck position for the specified library. Note that this assumes the plate is in a sensible location, as with “HeatingTemp”.

#### Associated Tags

Processing (required)

### B.2.6 Tare

#### Usage (Herman)

When set to “1” the given vials will be tared. The next call to “Weigh” will compare against this value.

Typically only used when explicitly weighing vials for a liquid dispense or when noting the mass of a vial over time.

#### Associated Tags

Processing (required)

### B.2.7 WaitForTimer

#### Usage (Herman)

Requires that “SetTimer” has been called previously. Blocks execution of maps until the timer has reached its end.

#### Associated Tags

Processing (required)

### B.2.8 Weigh

#### Usage (Herman)

When set to “1” the given vials will be weighed. If “Tare” has been used previously, the difference between the tare weight and the current weight will be reported.

Typically only used when explicitly weighing vials for a liquid dispense or when noting the mass of a vial over time.

#### Associated Tags

Processing (required)

### B.2.9 VortexRate

#### Usage (Herman)

Sets the vortex rate at the deck position for the specified library. Note that this assumes the plate is in a sensible location, as with “HeatingTemp”.

#### Associated Tags

Processing (required)