ESCALATE v3 UI User Guide

## 

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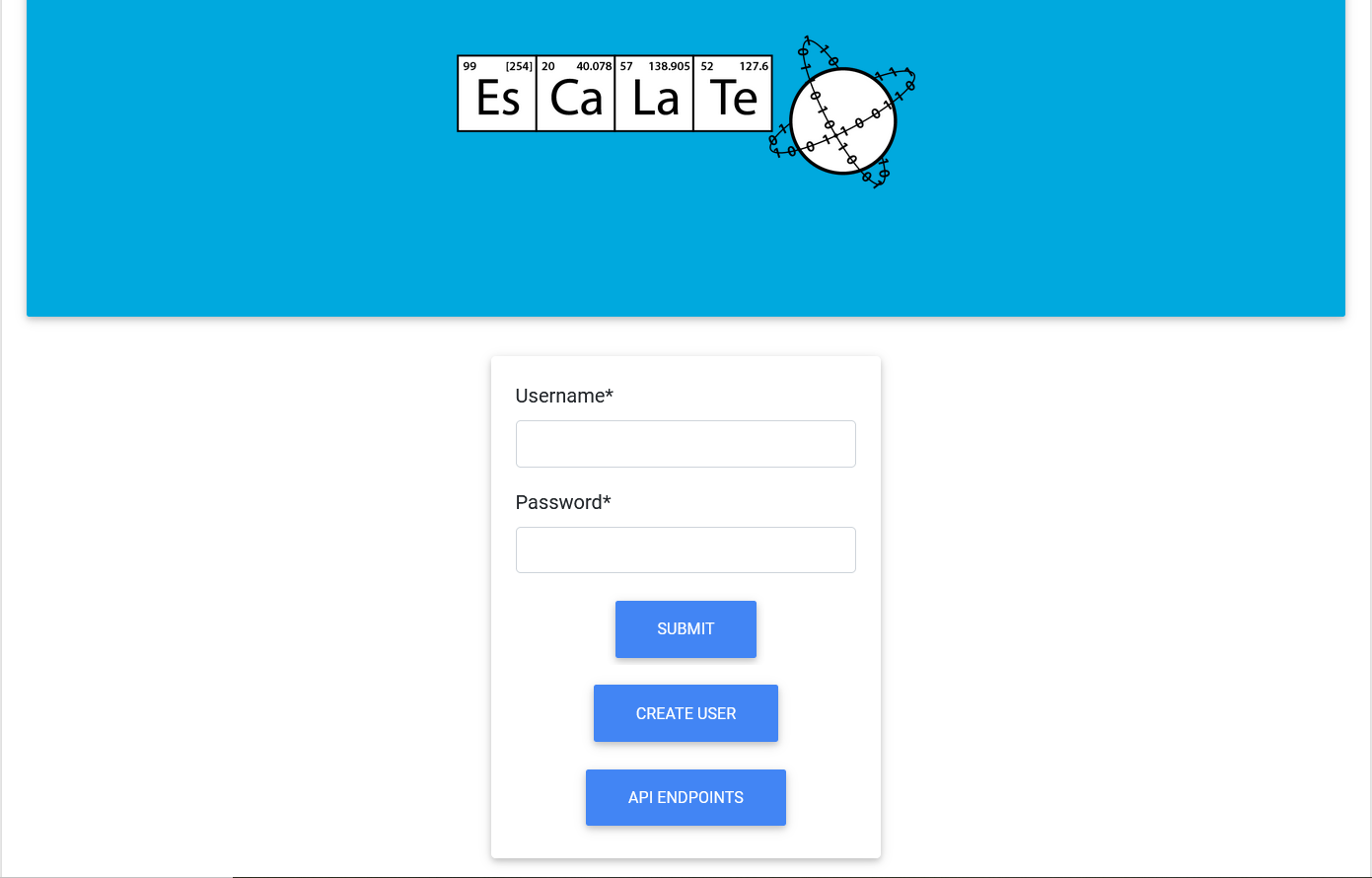
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## 

## **1. Introduction**

The purpose of this document is to guide new users through the ESCALATE v3 graphical user interface. Use the links in the table of contents above and throughout the user guide to quickly navigate through this document. For a detailed explanation of the API, reference the ESCALATE v3 API User Guide.

## **2. Account Creation/Login**

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### 2a. Account Creation

Navigate to the login page (localhost:8000 by default on local machine installations). Select the “Create User” button at the bottom of the page. This will cause the user creation form to populate the page. Fill in the required fields, marked with an (\*). Passwords can’t be too similar to personal information, must contain at least 8 characters, can’t be entirely numeric, and can’t be commonly used passwords.  
  
 Below the required fields are personal information fields. These fields will be used to pre-populate the user profile. These fields can be added/edited at any time from the [profile dropdown](#_cpybc7u8g2me) at the top of the main page.

Once a user has filled out the required fields and any personal information they would like to add at this point in time they can select the “Submit” button to process the form and create the user account.

### 2b. Login

At the login screen, fill in the username and password associated with an account and select “Submit”. Users with valid credentials will be redirected to the main menu. If you do not remember your credentials to log into the application please reach out to the administrator that is managing the ESCALATE application.

## **3. Main Menu**

A picture containing website

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*Dropdowns are labeled according to the sections below*

### 3a. Lab Selection/User Profile/Logout

Selecting your name in the top right corner of the application will open a dropdown menu with three options: “Select a lab”, “Profile,” and “Logout.”

Selecting “Select a lab” will navigate to the lab selection form, where you can select a lab organization from the drop-down menu. This is necessary before any experiment creation or template creation task. Note that labs are pre-populated via the API, and you must join a lab through the user profile before you can select that lab. Once you select a lab from the dropdown menu and press the “Select lab” to confirm your selection, the lab you’ve selected wil display in the navigation bar.

Selecting “Profile” will bring up your personalized user profile where you can see and edit personal information, add an image, and update lab associations. To join/leave a lab you must provide an organizational password that should be provided by that lab's administrator. Selecting “Logout” will log out of the application and redirect you to the login page.

### 3b. Inventory Dropdown

This dropdown provides a list of database elements that pertain to materials and chemical inventories. The corresponding database models can be viewed and edited, and a search bar is available to narrow results. More information about this functionality can be found in the next section: [Database Tables](#_4._Database_Tables).

### 3c. Tools Dropdown

This dropdown provides a list of database elements that pertain to tools and utilities. The corresponding database models can be viewed and edited, and a search bar is available to narrow results. More information about this functionality can be found in the next section: [Database Tables](#_4._Database_Tables).

### 3d. Experiment Dropdown

The experiment dropdown menu contains the main functionality of the UI application. Within this dropdown, you can access [experiment instance creation](#_twyqrc2b72zg), [the experiment queue](#_57vwhuoy4d4o), [the completed experiment list](#_57vwhuoy4d4o), and access to the [Escalation graphical software](#_6zkp2d4xprot). More detailed information will be provided in subsequent sections.

### 3e. Experiment Template Dropdown

The experiment template dropdown contains links for [experiment template creation](#_uvq256ym0a4), the list of existing templates, and access to database elements that might need to be modified for template creation purposes: Material Type, Property, Action Def, and Parameter Def. More detailed information will be provided in subsequent sections.

## **4. Database Tables**

In this section the functionality of exposed database tables is described. This applies to tables accessed via the “Inventory,” “Tools,” and “Experiment Template” dropdown menus.

Once you’ve selected a database table, you can view the entries, edit an entry, or search for a specific instance. You can also create a new entry using the green button labeled “Add” under the search bar.

Graphical user interface, text

Description automatically generated

### 4a. View

Initially all entries in the database table will be displayed in a list format, by default ordered by description for most of the models. The figure above shows part of this list for the Materials table. Any instances that need to be removed from the table can be deleted using the trash can button located in the rightmost column of the table. Any instance can be edited by selecting the pen and paper button in the rightmost column of the table. See [Section 4c: Edit](#_4c._Edit) for more information about editing the database table entries.

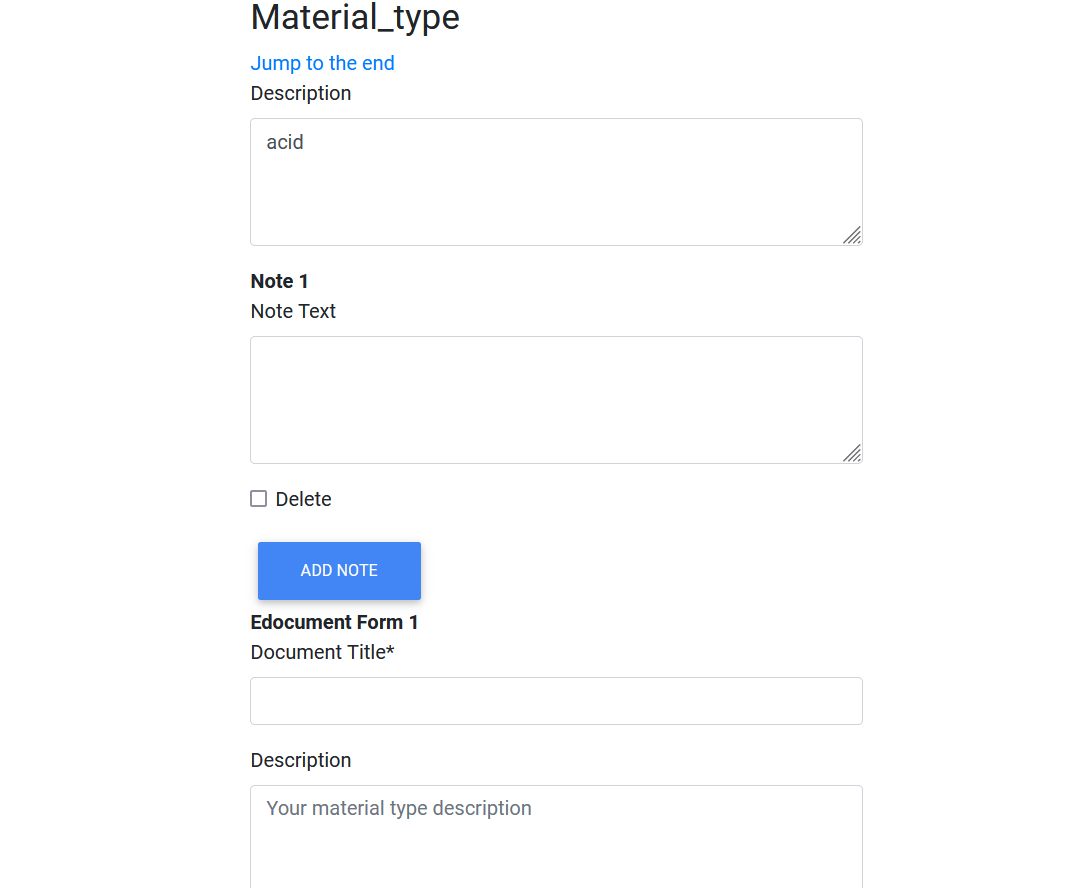
### 4b. Search

To narrow the results displayed or search for a specific instance, use the search bar at the top of the page.

### 4c. Edit

Below is a sample form that displays when you select the pen and paper button to edit an entry. The information available to edit will change depending on the database model being edited. Submit any altered information for a specific instance to save changes to the database.

Note that edit functionality is disabled for some models; for instance, experiment templates cannot be edited once they are used to create experiments.

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### 4d. Add New

To create a new entry for a database table, select the green “Add” button under the search bar. A form similar to the “Edit” form will display, except the different fields won’t be prepopulated. Filling out the form and pressing “Submit” creates a new database entry.

## **5. Create New Experiment Template**

Graphical user interface, text, application, email

Description automatically generated

New experiment templates can be created through the UI via the “Create Experiment Template” selection from the [experiment template dropdown menu](#_3d._Experiment_Template). An experiment template is associated with templates for reagents, vessels, outcomes, and actions. Once created, a template can be reused over and over for different experiments, and the specific parameters (e.g. chemical identity of materials in the reagents, temperature of a heating action) can be changed from experiment to experiment.

When you click “Create new experiment template” in the Experiment dropdown, the form shown above will be displayed. This form is used to name your template and declare the number of reagents, outcomes, and vessels. The text box labeled “Experiment Template Name” allows you to name the experiment template. Once your template is successfully created, this template name will show up in the dropdown menu in the [experiment creation](#_twyqrc2b72zg) process, allowing you to select the template for specific experiments. The text boxes labeled “Number of Reagents”, “Number of outcomes to measure”, and “Number of vessels used” take integer inputs corresponding to the desired number of reagents, outcomes, and vessels, respectively. For example, if the template is being used for experiments that involve two stock solutions and an acid, and you wish to record whether a product formed, you would enter “3” for the number of reagents and “2” for the number of outcomes. Presuming each of the reagents has its own container and you are dispensing them into another container during the course of the reaction, you would enter “4” for the number of vessels. Then, click the “Next Step” button to bring you to the next form (shown below), where you can specify details about the reagents.

Graphical user interface

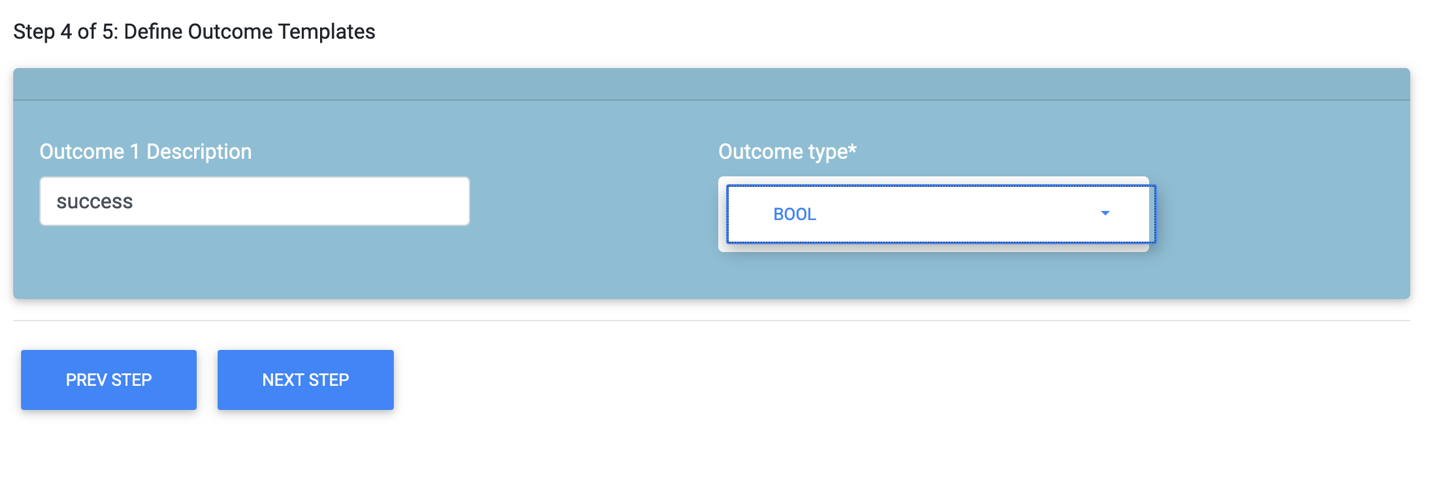
Description automatically generated

For each reagent, enter a name in the text box labeled “Reagent {i} Name” and enter an integer value corresponding to the number of materials (components) in that reagent in the “Number of Materials” box. Note that each reagent must contain at least one material. Use the drop-down menu to select properties that you would like to associate with the reagent as a whole. This will create property templates that link to the reagent template in the database. For example, suppose the stock solutions are being stored in beakers and the dead volume of the beaker is of interest to ensure that the right amount of solution is prepared. In this case, a dead volume property can be associated with the reagent. Multiple properties can be selected for the same reagent, if desired: hold down the command/ctrl key as you click on each of the desired properties. If a desired property is not listed in the dropdown, it can be created using the API or by selecting “PropertyDef” in the “Experiment Template” dropdown from the navigation bar and then clicking “Add new PropertyDef”, but note that this requires navigating away from experiment template creation and your changes will be lost. See the [Model](#_rk5l5an7yvv1) section for more information on adding a new property definition using the UI.

Once data has been entered for each reagent, click “Next step.” To change the number of reagent boxes that display on this page, press “Prev step” and modify the number entered in the “Number of Reagents” box in the previous form.

Graphical user interface

Description automatically generated

The following form (shown above) allows for specification of the material components that go into each reagent. For each reagent, the reagent name, entered on the previous form, is displayed for reference; it cannot be modified on this screen. Optionally, the drop-down menu can be used to select one or more material-level properties. This will create property templates that associate with each reagent material template in that reagent. Like in the previous form, multiple material properties can be selected for the same reagent, if desired: hold down the command/ctrl key as you click on each of the desired properties. Again, if a property is not listed, it can be added via the API or the UI but requires navigating away from the experiment template creation wizard. Boxes are then displayed to indicate the material type for each material in the reagent; the number of materials corresponds to the integer entered on the previous page. Select the desired material type from the drop-down menu. Like properties, material types can be added to the database if the desired type is not displayed in the drop-down menu. Again, this can be done through the API or by navigating to “MaterialType” under the “Experiment Template” dropdown and selecting “Add new material type”. Once the form is complete, click “Next step,” bringing you to the outcome definition form.

This form, shown above, allows you to specify the outcome(s) for the experiment template. For each outcome, you can define the name of the outcome as well as its data type. For instance, you might define an outcome called “Success” with a Boolean data type, allowing you to specify true or false for each experiment using the template. To change the number of outcome boxes that display on this page, press “Prev step” until you return to the first form and modify the number entered in the “Number of Outcomes” box, then return again to the outcome form using “Next step”. This will not delete or modify the data entered for the reagents or materials. Once data has been entered for each outcome, click “Next step.” This brings you to the final step of the experiment template form wizard.

Graphical user interface

Description automatically generated

The last step involves specifying the vessels to be used in the experiment template (see form above). For each vessel, you can add a description, select a default from the drop-down menu, and indicate whether it is an “outcome vessel.” The default vessel is a placeholder and can be changed when the template is used for experiment creation. If the “outcome vessel” box is checked, this is the vessel that will be used to generate labels for outcome-related files. For instance, if you are dispensing stock solutions into a collective flask and then noting whether crystals grow once all the stocks are mixed for your outcome, the containers that hold the stock solutions are NOT outcome vessels because they have no relevance to the outcome you are measuring. The flask will be an outcome vessel because this is the vessel you are referencing when measuring outcomes.

Once the vessel specification form is completed, press “Next step.” This submits the data you have entered to create a template and associate that template with the reagents, outcomes, and vessels you have specified. In case of errors validating any of the forms, you will be redirected to the form that needs to be corrected to modify the problematic inputs. Once the template has been successfully created, you will be redirected to a page with a link to a workflow designer that can be used to generate action templates. Note that the template is not considered complete and cannot be used to create experiments until action templates are associated with it.Diagram

Description automatically generated

Once you navigate to the workflow designer page, which is shown above, you can define one or more action templates. Each action template describes a step in your experimental procedure, and it consists of an action definition, a source vessel, and a destination vessel. Use the “Add action” button to view and select from the list of action definitions. If there are missing action definitions, they can be added via our API endpoint ActionDef or, more conveniently, by selecting “Create new action def”. This button opens a pop-up window (shown below) in which you can enter the description of your desired action definition and select the parameters you wish to record. For example, suppose part of your workflow requires letting a vessel cool for a certain amount of time or until it reaches a certain temperature. To define this action def, you might enter “cool” as the description and then select “temperature” and “duration” for the parameters. Multiple parameters can be selected by holding down the command/ctrl key as you click on each of the desired parameters. Press “Save” to save the action def.

Graphical user interface, application

Description automatically generated

Once you select an action definition, a box will appear on the screen with the action definition’s description (see visual below).

**Graphical user interface, text, application, email

Description automatically generated**

Click on the box to edit the description, source and destination. Follow these conventions:

* If an action is being performed on a single vessel (for example, heating a well plate), leave the “From” box blank. There will be no source. In the “To” box, select the appropriate vessel template. This will be the destination.
* If an action involves a transfer of a material from one vessel into another (for example, dispensing), select the appropriate vessel that will be transferred in the “From” box; this will be the source. In the “To” box, select the appropriate vessel template which the contents will be transferred. This will be the destination.
* If an action applies to a decomposable vessel (i.e. the wells inside of a well plate), check the checkbox labeled “Destination vessel decomposable?”

When you are finished editing the action, press “Save” to return to the main workflow designer screen.

Connect the action templates in the appropriate order for your experimental procedure. To connect them, drag and drop the arrows between the boxes. Note that, in order for your workflow design to be valid, it must begin with the “Start” node and end with the “End” node. These show up by default on the screen but can also be accessed and added via “Add action.” When you are finished, press the “Save” button. This will create an action template for each box and associate them with the experiment template.

If you would like to start over, use “Clear All Actions” to clear the action boxes. Note that workflow designs will not be saved when cleared unless you have pressed “Save”. Note also that creating a new design and pressing “Save” overwrites the previous one. In other words, although many action templates can be associated with an experiment template, they must all be created at once with a single workflow design.

Once you associate your action template with the experiment template by pressing “Save,” the experiment template is considered complete and can be used to create experiments. If you made an error and need to edit the experiment template in any way (e.g. adding or removing a reagent, reordering action templates, etc), select “View Templates” under the “Experiment Template” dropdown menu, navigate to the “Actions” portion of the table, and click the “Edit” button. Editing a template is only possible BEFORE the template is used for experiment creation; once experiments are created, a template cannot be modified.

## **6. Experiment Creation**

Experiments can be created via the “Create Experiment” selection from the [experiment dropdown menu](#_5lx71huup1iz). Once this is selected, you will be redirected to a multi-step form wizard. Details for each step are provided in each subsection below.

### Step 1: Select Experiment Template

Rectangle

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The first form in the wizard is similar to the form displayed above. This form allows you to specify a name for your experiment and to select an [experiment template](#_uvq256ym0a4). The dropdown menu for experiment template selection is prepopulated with all previously created templates (as described in the previous section) that are associated with your lab/organization.

### Step 2: Select Vessels

Graphical user interface

Description automatically generated

Step 2 (see form above) involves the selection of vessels. A colored box with a dropdown menu is displayed for every vessel template associated with the chosen experiment template. Use the dropdown menu to select your desired vessels.

Note that each vessel template has a default, specified at the template level, but on this screen you are able to select the actual vessel being used for this particular experiment instance. This means that you do not always have to use the same vessels from experiment to experiment, even if you are using the same template, allowing for more flexibility of inputs.

### Step 3: Specify Reagent Parameters

Chart, bar chart

Description automatically generated

Step 3 (a portion of the form is displayed above) allows you to specify values for all properties associated with each reagent, as well as with all the materials within each reagent. There is a colored box for each reagent. Reagent-level properties appear at the top. For each property, enter the desired value and unit, and select a type from the dropdown. Note that these are not required, so the values you enter depend on your experimental needs. However, if values are entered they must be chemically and numerically sound, e.g. the form will be returned with an error if you enter a negative number into an “amount” field.

Then, there are tabs that can be used to navigate through the materials. Each tab contains a dropdown list used to select a material, as well as value fields to update material-level properties. Selection of a material is required; the dropdown is populated based on materials within the database’s inventory and includes all materials tagged with the material type indicated for the experiment template. Material-level properties, like reagent-level properties, are optional, not required.

### Step 4: Specify Action Parameters

Step 4 allows you to specify parameter values for all actions in your experimental procedure that are not decomposable. Parameter values that apply to decomposable actions can be specified in [step 6,](#_6f._Step_6) described below. Colored boxes are displayed for each action and contain value fields for each of the parameters. Values and units can be entered, and the type can be selected from the dropdown. Again, inputs are validated, so they must be chemically and numerically sound.

### Step 5: Specify Automated Experiments

Graphical user interface, application

Description automatically generated

Step 5 (see form above) asks for the number of “automated” experiments you would like to run. “Automated” means that a sampling algorithm will be used to generate data. Sampling algorithms can be added to the codebase as plug-ins. By default, ESCALATE contains plugins for random samplers that can determine different volumes of each reagent to dispense into an outcome vessel (e.g. wells of a well-plate) that fall within the sample space of the convex hull defined by reagent concentrations. See doi i:10.1021/acs.jchemed.0c01456 for more information about this algorithm.

For “Number of Automated Experiments” type an integer greater than or equal to 0. Then, if you entered a number greater than 0, use the dropdown menu to select the appropriate sampler plugin.

Note that, if a sampler is selected and there are required user inputs to run it, the next form will display the variables that require user input and prompt you to enter values.

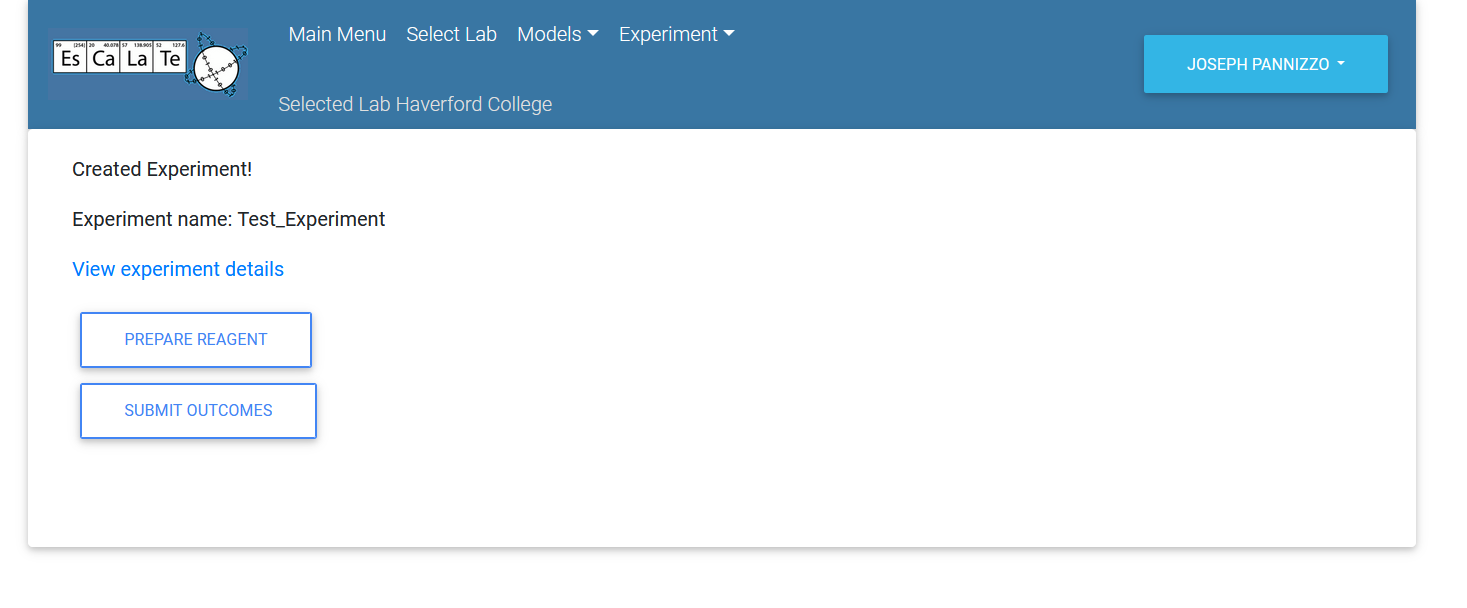
### Step 6: Specify Manual Experiments

Step 6 asks for details about decomposable actions. For instance, if your experiment involves dispensing a stock solution into certain wells of a well plate, you would specify the details for the parameters of the dispense action (e.g. volume to be dispensed). Click the blue hyperlink to download an excel file with a list of all the decomposable actions organized by vessel (rows) and reagent (columns). Fill in the desired values accordingly. This is called “manual” experiment specification because you are manually filling in the file. Once complete, save the Excel spreadsheet onto your computer and then use the “Browse” button to search for and upload the file.

Note that this step is optional and a file need not be uploaded if you are not manually specifying experiments. If there are no decomposable actions (as is the case for the demo template we are using), the file will be blank. Note also that if you are running automated experiments, data generated by the sampler will show up in the downloadable file and it can be manually overwritten at this step.

### Step 7: Select Postprocessors

The last step of experiment creation is optional and allows you to select postprocessors. These are plugins that can run calculations on your experimental data. For instance, ESCALATE contains a plugin that can calculate amounts of each material to add to a reagent so that you obtain solutions of desired concentrations. You can add your own plugins to the codebase if applicable.

Upon successful completion of all steps of the form wizard, you will see a confirmation screen similar to the one below. There will be buttons/links to the [experiment details](#_yuejfc8r3pvm), [reagent preparation](#_x39appsy4fom), and [outcome](#_kr9tb93y6q11) forms for the experiment that was created. These forms will be detailed in the [Experiment Queue/Completed Experiment List](#_57vwhuoy4d4o). 

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Below the manual file upload will be a list of reagents associated with the experiment template. The desired concentrations for each chemical within the reagent should be populated; the unit of measurement by default is molarity (moles/Liter) and should be updated if it is different from the default. **Note:** The concentration values must be non-negative numbers. Technically, the concentration value for a solvent is meaningless and therefore can be left as 0.0 M, but the experiment creation process will function as long as any non-negative number is entered and the values for solvent concentration will simply be ignored.

This experiment creation process, unlike manual experiment creation, does not rely on a file upload. Functionally, the rest of the experiment creation form is the same as detailed within the [manual experiment creation](#_lkfplextmaqz) process.

This will redirect you to the automated experiment specification form. At the top of the screen you will be required to name the experiment instance. Below this will be a list of reagents associated with the experiment template. The desired concentrations for each chemical within the reagent should be populated and the unit of measurement should be updated if it is not being measured in moles. **Note:** All non-solvents should contain a non-zero, positive number.

## **7. Experiment Queue/Completed Experiment List**

Both the experiment queue and completed experiment list operate similarly. They can both be accessed from the [experiment dropdown](#_5lx71huup1iz) at the top of the page. The experiment queue tracks pending and running experiments while the completed experiment list tracks finished experiments. **Note:** Invalidated experiments will not be tracked by either list but can be accessed via the API. Experiments that are deleted are marked as invalid and are not removed from the database.

### 7a. Edit Experiment



Using the button with a pen and paper icon, a user can edit parameters, change the status of an experiment, upload e-documents, and change the priority of an experiment. An in-depth explanation of this experiment detail editor can be found in the [Experiment Detail Editor](#_yuejfc8r3pvm) section.

### 7b. Outcome



The outcome section is used at the completion of an experiment to provide results relevant to that experiment instance. The outcome form provides a file download that can be populated and re-uploaded using the file browser within the outcome form. Any relevant files, images, spectroscopic results,, etc. can be uploaded using the second file browser below the outcome upload to attach any associated information relevant to the completed experiment. Once the relevant files are uploaded select the “Submit” button to upload the files to the database. Custom outcome files can be created through our Outcome API endpoint and will be associated with the relevant experiment template.(*A full list of our exposed API endpoints can be found at localhost:8000/api/ for local installations*)

### 7c. Reagent Preparation



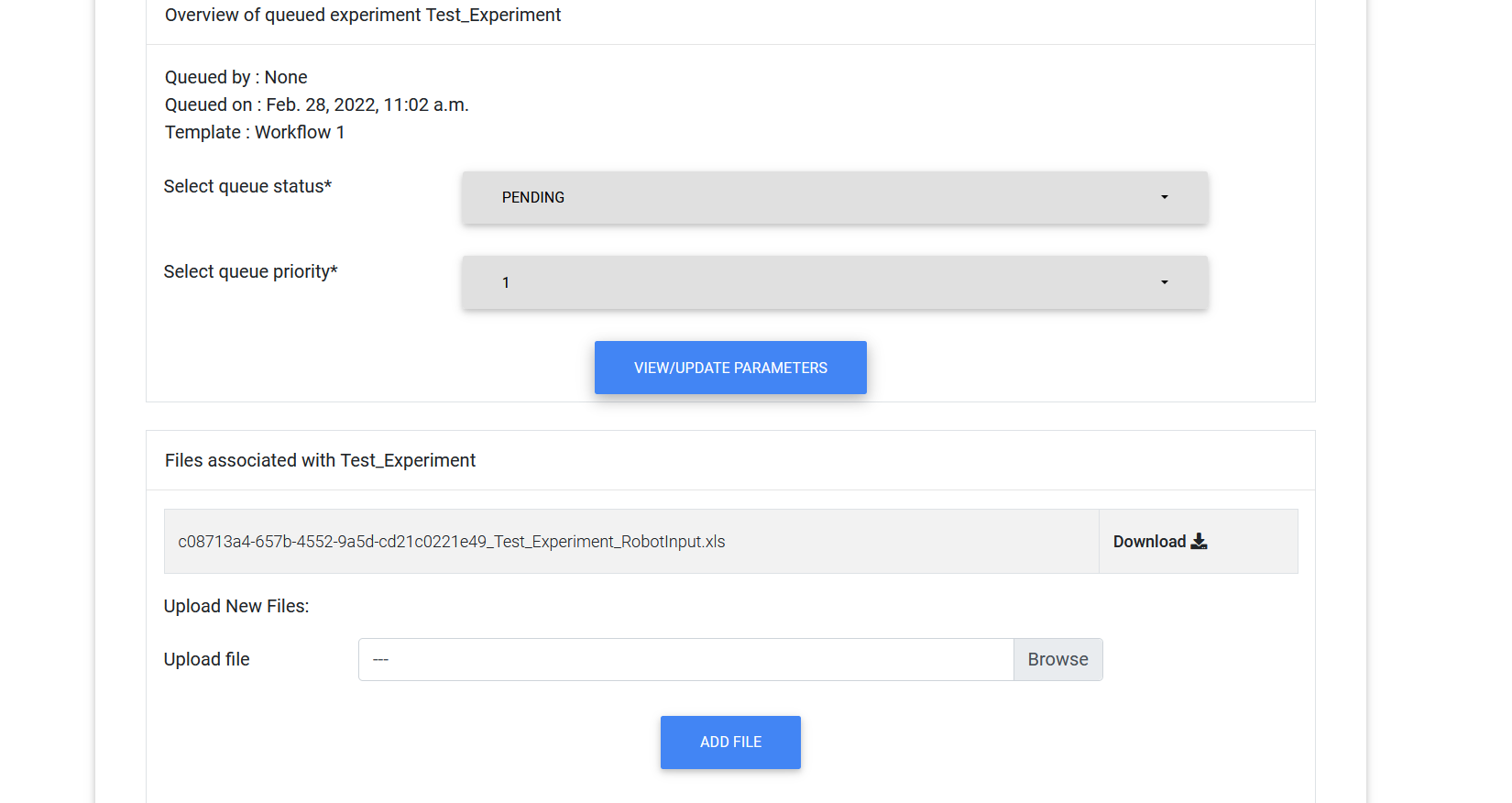
Reagent preparation is used to report the actual values of the chemicals used within the desired experiment. The nominal values will be pre-populated based on the manual input file that was uploaded during the [experiment creation process](#_twyqrc2b72zg), our automated reagent preparation algorithm, or both depending on how the experiment was created. The reagent preparation form provides input fields for the actual values that should be filled out in its entirety. The units of measurement should be updated as well if the default units of measurement are not applicable. To submit user changes click the “Prepare Reagents” button at the bottom of the screen.

### 7d. Delete

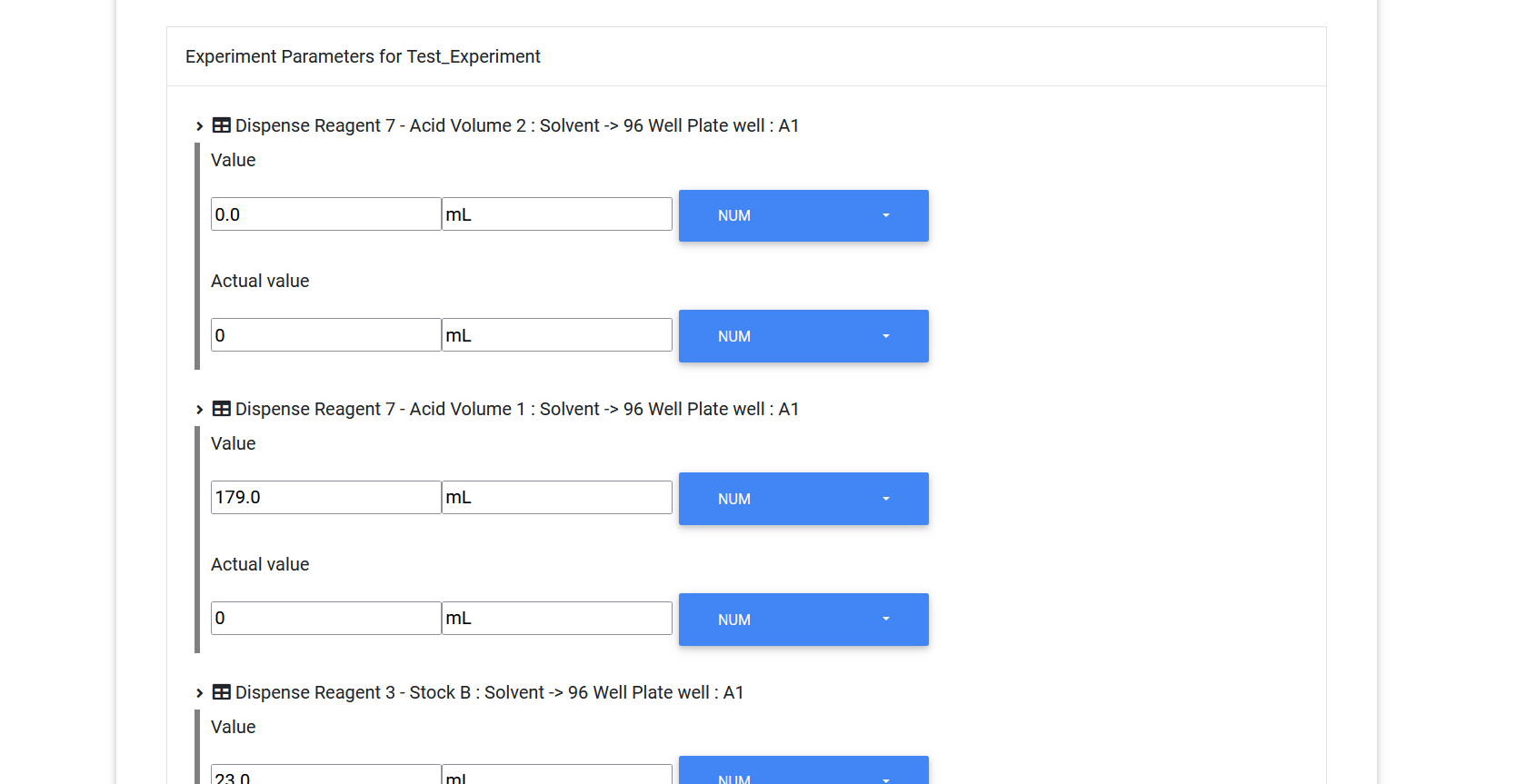


The delete button is used to invalidate any experiment instance. In order to maintain a persistent record of all experiment instances we do not remove deleted experiments from our database. Instead we set the status of those experiments to Invalid and they are removed from both the [experiment queue](#_57vwhuoy4d4o) and [completed experiment list](#_57vwhuoy4d4o). When the delete button is selected the user will be prompted to confirm deletion (i.e., setting the status to invalid) before the experiment instance is removed from the list.

## **8. Experiment Detail Editor**



The experiment detail editor provides an overview of an experiment instance and the means to update any incorrect values within that experiment. Within this screen you can view the current status of the experiment, parameter information, and associated e-documents. The first section in the experiment detail editor provides an overview that allows the user to select the priority and update the status of the experiment. Any changes to this section needs to be submitted using the “Update Experiment” button at the bottom of the page. The button below the queue priority, View/Update Parameters, allows a user to update experiment parameters. Selecting this button will redirect you to a form similar to the image below. Each parameter associated with the experiment can have its nominal and actual values bulk updated by inserting the new values and selecting “Update Parameters” at the bottom of the page. Once the form is processed you will be redirected to the experiment details page once again.



Below the parameter update button is a section that allows a user to upload and view files associated with the experiment. To download and view a file that exists on the system simply click the “Download” button to the right of each e-document. To upload a file select the “Browse” button and select the corresponding file in the file explorer. Once that file is selected click the “Add File” button at the bottom of the page.

## **9. Escalation**

Escalation is a web application developed by TwoSix Labs that generates graphical representation of data that can be found within ESCALATE. Escalation has its own documentation and working examples provided by TwoSix Labs located [here](https://github.com/twosixlabs/Escalation).

## **10. References**

Below are a list of useful external references:

* [Escalate v3 General Readme](https://github.com/darkreactions/ESCALATE/blob/master/escalate/README.md)
* [Escalate v3 Technical Readme](https://github.com/darkreactions/ESCALATE/blob/master/escalate/TECHNICAL.md)
* [Escalate v3 Data Model Readme](https://github.com/darkreactions/ESCALATE/blob/master/data_model/README.md)
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