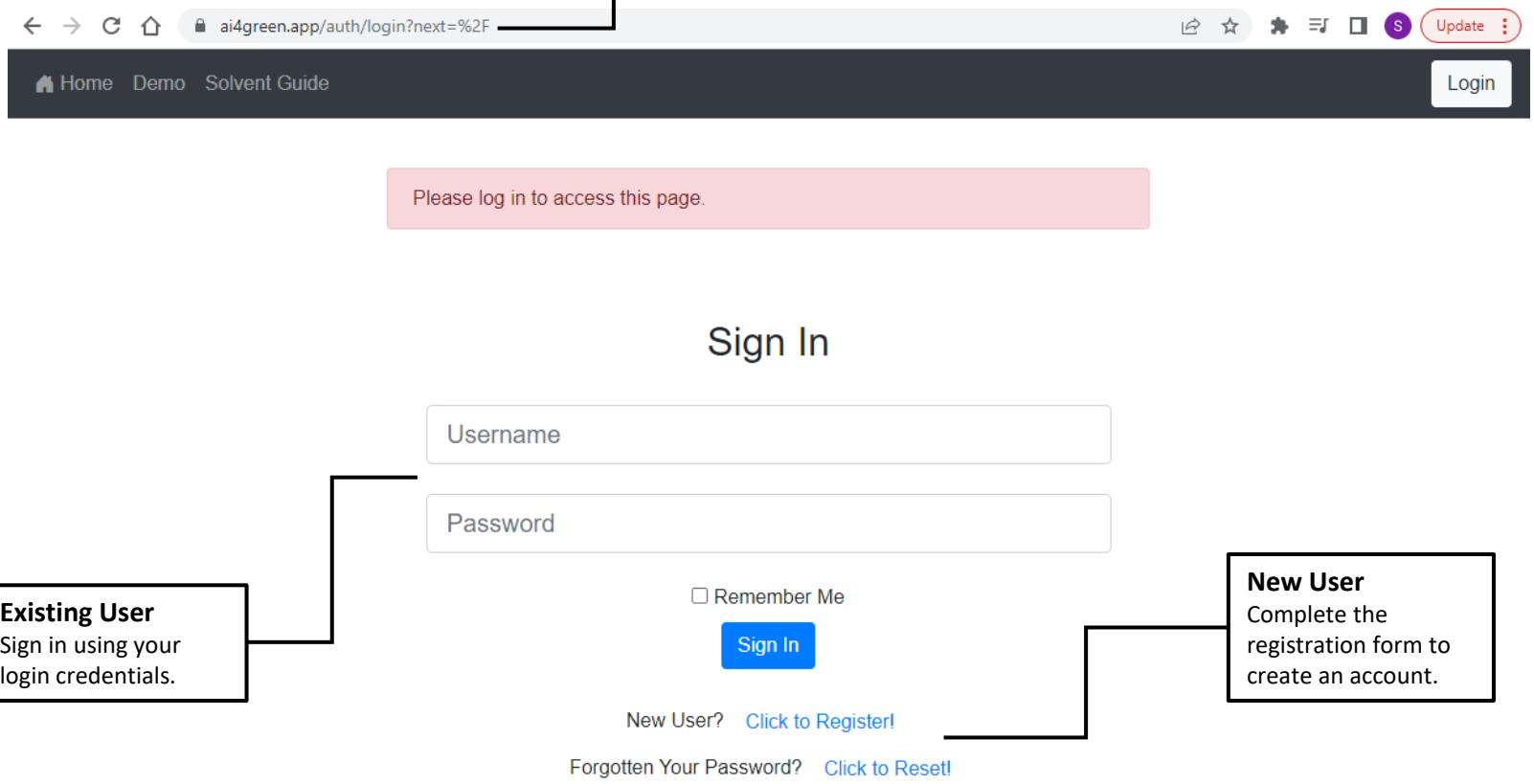
Accessing AI4Green

Web Browser
We recommend using Google Chrome.

URL
Type in 'ai4green.app' into the address bar.



Existing User
Sign in using your login credentials.

New User
Complete the registration form to create an account.

Getting Started

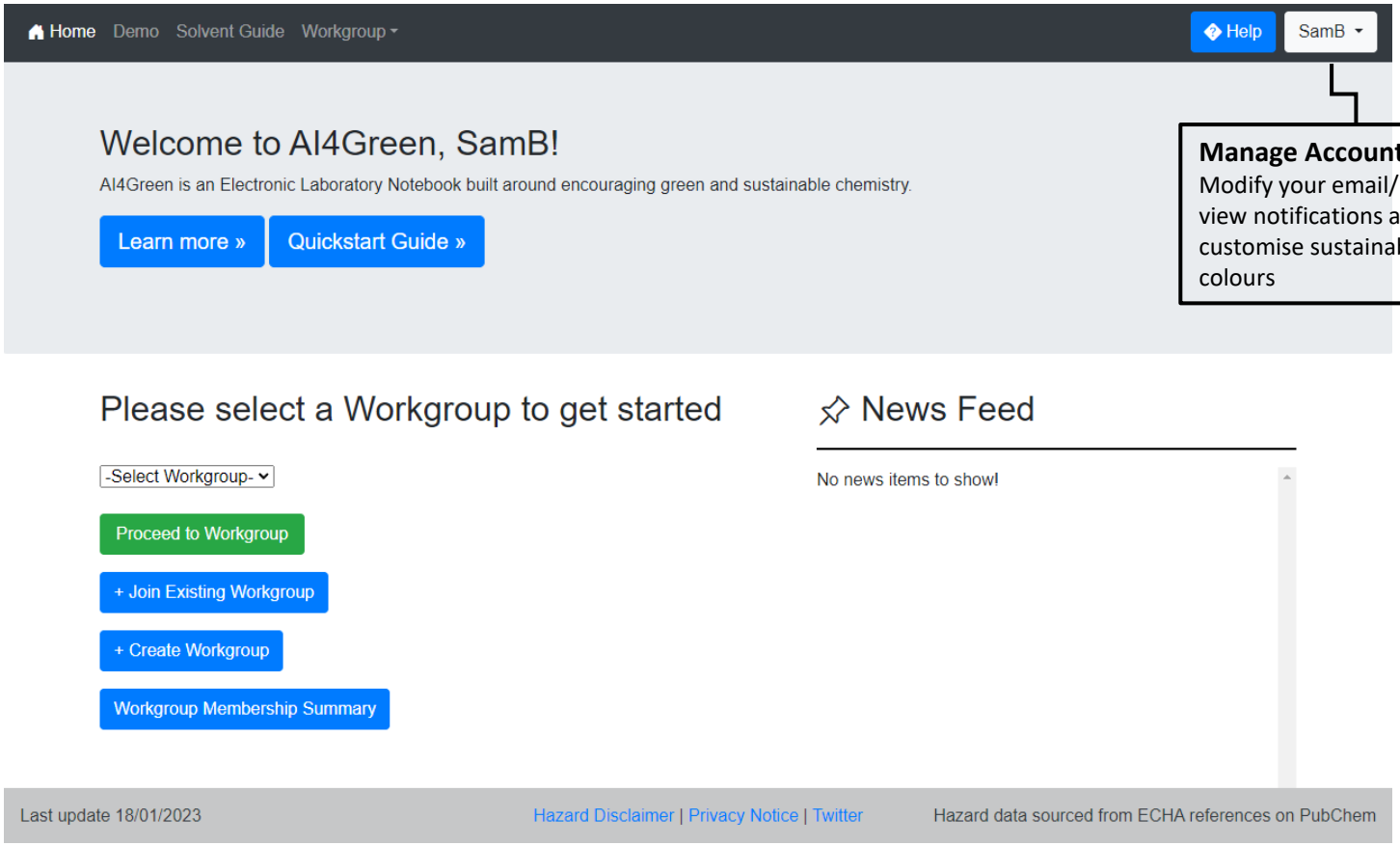
Demo
Try a limited version of the reaction constructor before joining a workgroup.

Solvent Guide
Access our sustainable Solvent Guide.

Workgroup
Quick access a Workgroup.

Help
Access our help guides and video tutorials.

Home
This is the home page.



Manage Account
Modify your email/password, view notifications and customise sustainability colours

Workgroups
You must join or create a workgroup to access the complete functionality.

Join Workgroup
If your research group has already made a workgroup, you can request to join this workgroup

Create Workgroup
If you are the principal investigator or equivalent, you can apply to create a workgroup.

Getting Started – Principal Investigators

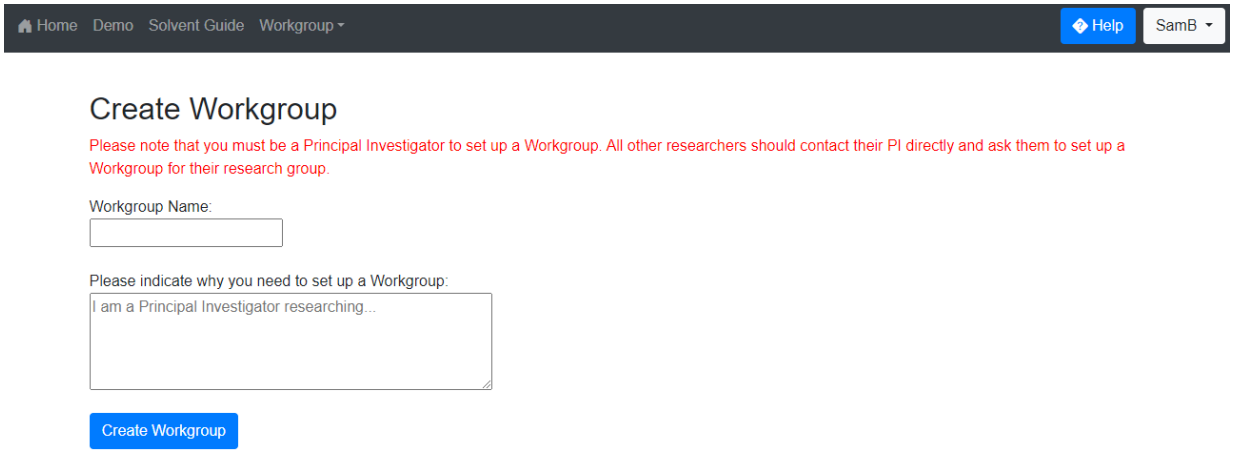
1 Create Workgroup

This is the create workgroup page.

If you are a principal investigator you will be able to create and use a workgroup immediately by completing the form on this page.

Once created other registered users will be able to see the workgroup and request to join.

You will receive an email when a request is made and all requests will be shown on the notifications page where they can be approved or denied.



2 Create Workbook

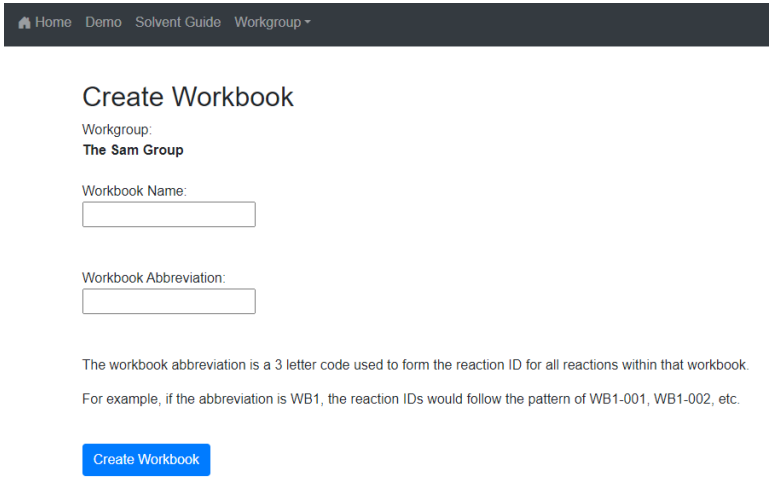
This is the create workbook page

A workbook is designed to act as a collection of all researchers & reactions associated with a particular project. A workgroup can have multiple workbooks. Users must belong to a workbook & workgroup before they can start creating reactions. Senior researchers can also create/manage workbooks.

If you are a principal investigator you will be to add users to workbooks on the **manage workbooks** page.

You will also be able to change workgroup members usertype on the **manage workgroup** page.

These actions can also be done by approving user requests.



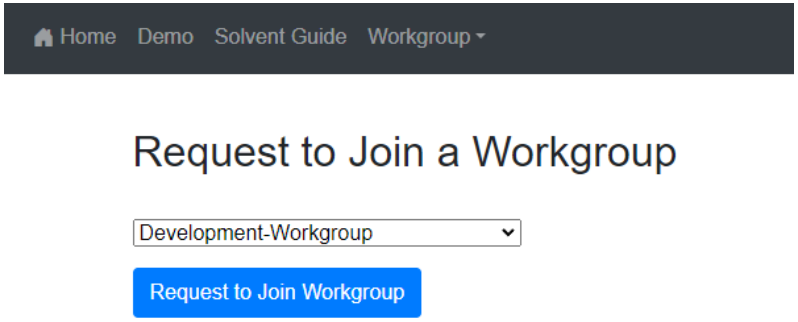
Getting Started – Standard users

1 Join workgroup
This is the join workgroup page.

You should join the workgroup of your principal investigator.

To do this find their workgroup from the dropdown and then select and request to join the workgroup.

The principal investigator of the workgroup will then receive a notification and approve or deny the request.

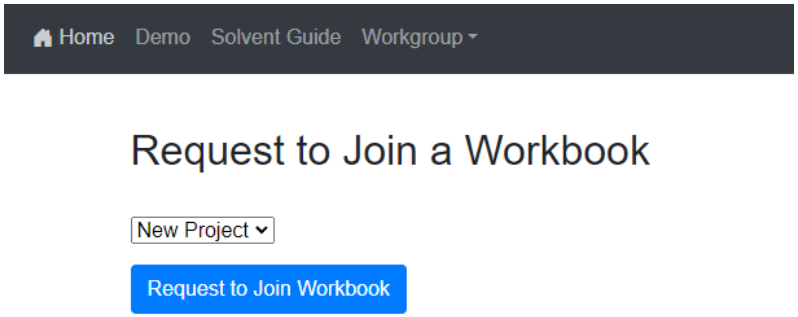


2 Join workbook
This is the join workbook page

Once you a workgroup member you will have access to the workgroup page where you will be able to join workbooks by request or having your PI add you directly.

Your usertype can also be changed by your PI or you can make a request. Senior researchers are able to create and manage workbooks.

You must belong to a workbook within a workgroup before you can create reactions.

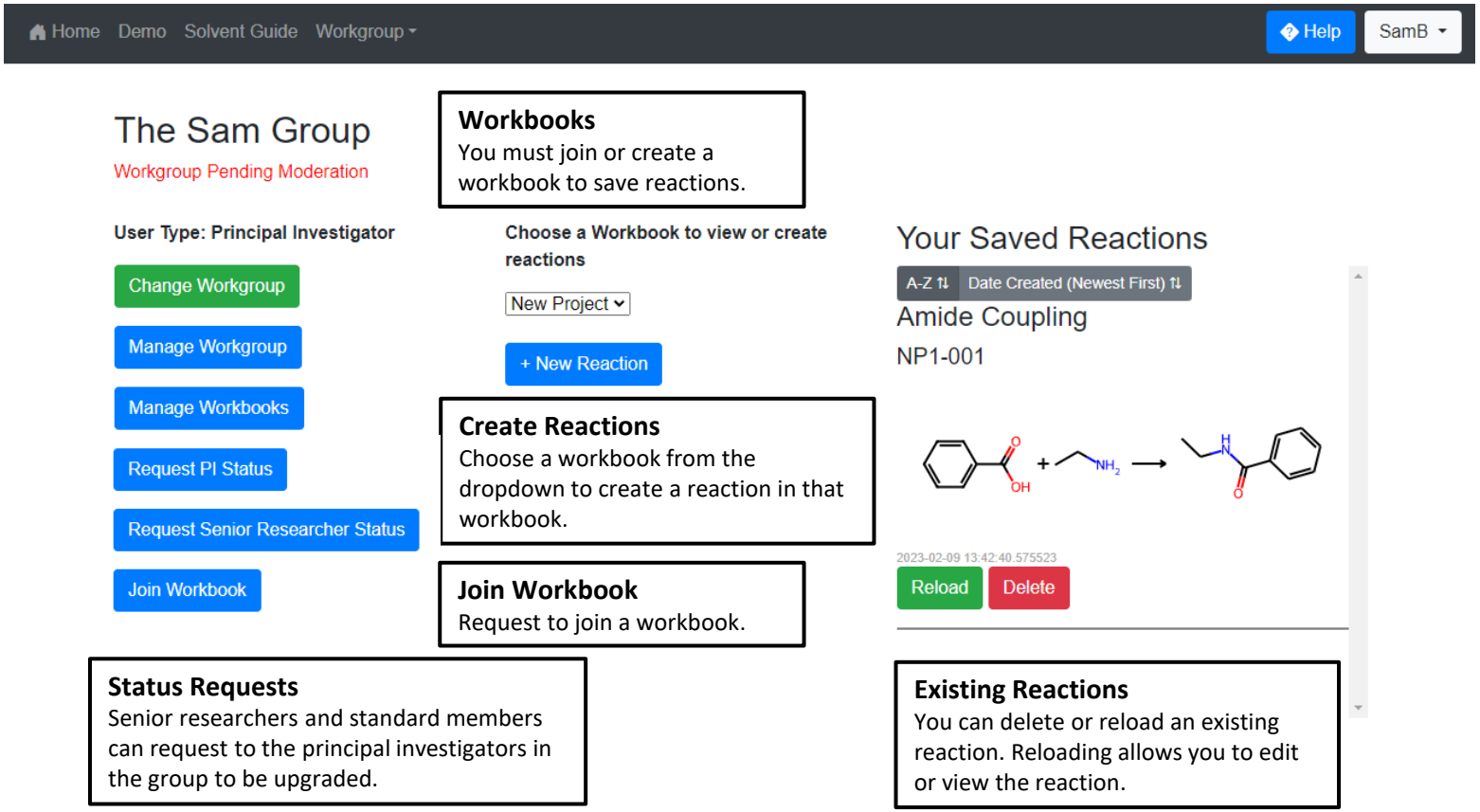


Workgroups

Workgroup page
This is the workgroup page. A workgroup contains multiple workbooks & users.
Visible buttons depend on user type and may differ from those shown.

User type
Within a workgroup, users are classed as a standard member, senior researcher or principal investigator.
A user can be in multiple workgroups and have a different role in each.

Management Pages
Principal investigators can manage the workgroup membership and usertypes.
Principal investigators and senior researchers can manage workbook membership.



Workbooks
You must join or create a workbook to save reactions.

Create Reactions
Choose a workbook from the dropdown to create a reaction in that workbook.

Join Workbook
Request to join a workbook.

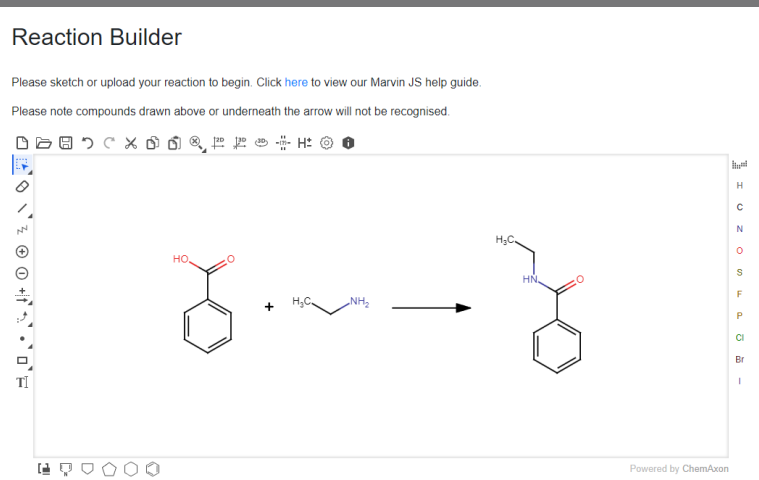
Status Requests
Senior researchers and standard members can request to the principal investigators in the group to be upgraded.

Existing Reactions
You can delete or reload an existing reaction. Reloading allows you to edit or view the reaction.

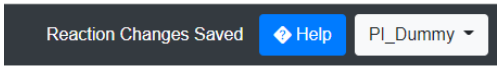
Reactions

1 Sketcher
Draw the reaction in here.
Compounds drawn over the arrow will be ignored.
Press “Submit” to continue.

2 Reaction Table
Fill in all highlighted boxes.
Add any reagents or solvents by CAS or name.
New compounds can be added to database.
Press “Summary” to proceed.



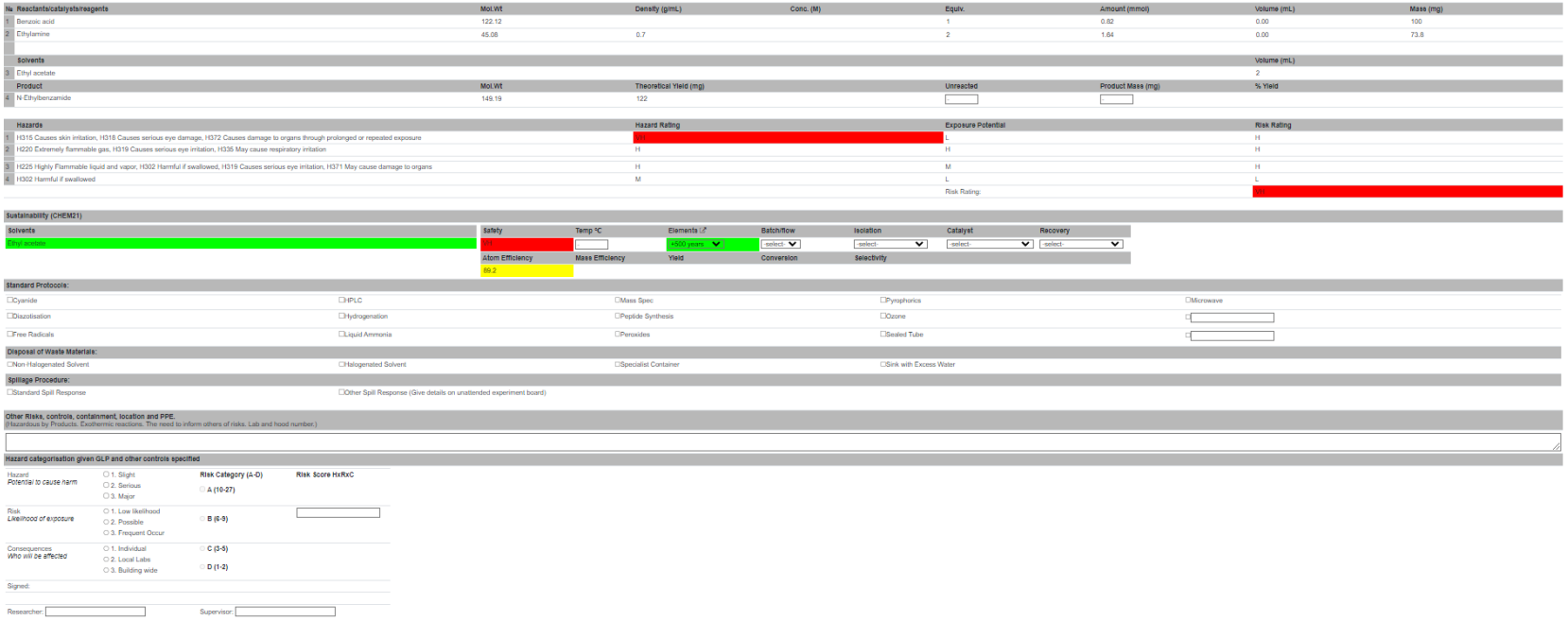
Autosave
All data entered into the reaction will be autosaved. Upon each successfully saved change, the message shown below will display in the top right of the screen.



Reload
A reaction can be reloaded at any stage from the saved reactions list.

Reactions 2

3 Summary
Fill in all the fields you can. You can reload and add further information later.



№	Reactants/catalysts/reagents	Mol.Wt	Density (g/mL)	Conc. (M)	Equiv.	Amount (mmol)	Volume (mL)	Mass (mg)
1	Benzoic acid	122.12			1	0.82	0.00	100
2	Ethylamine	45.08	0.7		2	1.64	0.00	73.8

	Solvents	Volume (mL)
3	Ethyl acetate	2

	Product	Mol.Wt	Theoretical Yield (mg)	Unreacted	Product Mass (mg)	% Yield
4	N-Ethylbenzamide	149.19	122			

	Hazards	Hazard Rating	Exposure Potential	Risk Rating
1	H315 Causes skin irritation, H318 Causes serious eye damage, H372 Causes damage to organs through prolonged or repeated exposure	VH	L	H
2	H220 Extremely flammable gas, H319 Causes serious eye irritation, H335 May cause respiratory irritation	H	H	H
3	H225 Highly Flammable liquid and vapor, H302 Harmful if swallowed, H319 Causes serious eye irritation, H371 May cause damage to organs	H	M	H
4	H302 Harmful if swallowed	M	L	L
			Risk Rating:	VH

Sustainability (CHEM21)

Solvents	Safety	Temp °C	Elements	Batch/flow	Isolation	Catalyst	Recovery
Ethyl acetate	VH		>500 years	-select-	-select-	-select-	-select-

Atom Efficiency	Mass Efficiency	Yield	Conversion	Selectivity
89.2				

Standard Protocols:

☐Cyanide	☐HPLC	☐Mass Spec	☐Pyrophorics	☐Microwave
☐Diazotisation	☐Hydrogenation	☐Peptide Synthesis	☐Ozone	☐
☐Free Radicals	☐Liquid Ammonia	☐Peroxides	☐Sealed Tube	☐

Disposal of Waste Materials:

☐Non-Halogenated Solvent	☐Halogenated Solvent	☐Specialist Container	☐Sink with Excess Water

Spillage Procedure:

☐Standard Spill Response	☐Other Spill Response (Give details on unattended experiment board)

Other Risks, controls, containment, location and PPE.
(Hazardous by Products. Exothermic reactions. The need to inform others of risks. Lab and hood number.)

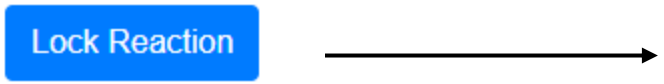
Hazard categorisation given GLP and other controls specified

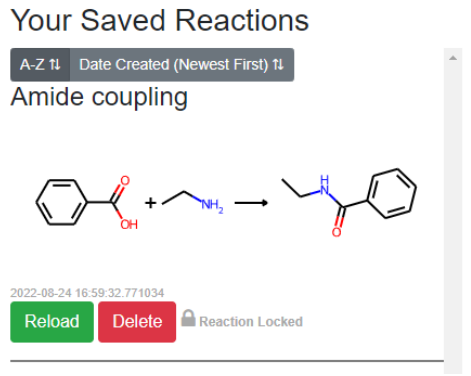
		Risk Category (A-D)	Risk Score HxRxC
Hazard *Potential to cause harm*	○ 1. Slight ○ 2. Serious ○ 3. Major	○ A (10-27)	
Risk *Likelihood of exposure*	○ 1. Low likelihood ○ 2. Possible ○ 3. Frequent Occur	○ B (6-9)	
Consequences *Who will be affected*	○ 1. Individual ○ 2. Local Labs ○ 3. Building wide	○ C (3-5) ○ D (1-2)	

Signed:

Researcher: Supervisor:

4 Locking
Once the reaction is complete and you do not wish to make more changes, click the “Lock Reaction” button.
The reaction is now locked for editing but can still be viewed.





Additional Information

This guide has focused on the key steps required for a new user to use our core ELN functionality as quickly and smoothly as possible.

There are additional tools within our web app, such as green metrics and sustainable solvent selection guide.

There are also other important features you will encounter, such as notifications and workgroup and workbook management.

For further information on these go to the help page (button in the top navigation bar) to find our full user manual.