Accessing AI4Green

Web Browser
We recommend using Google Chrome.

URL
https://ai4green.app/

Existing User
Sign in using your login credentials.

New User
Complete the registration form to create an account.

Welcome to AI4Green

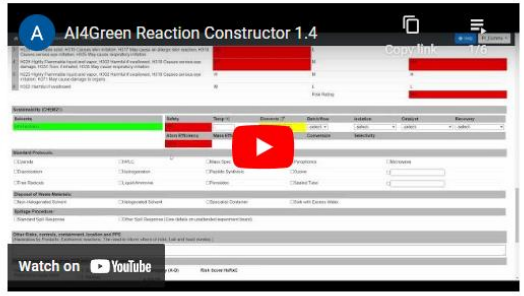
AI4Green provides an ELN including collaboration tools, data archival and management and green and sustainability metrics for organic chemistry.

It is accessible via a web interface and fully available on an open source basis.

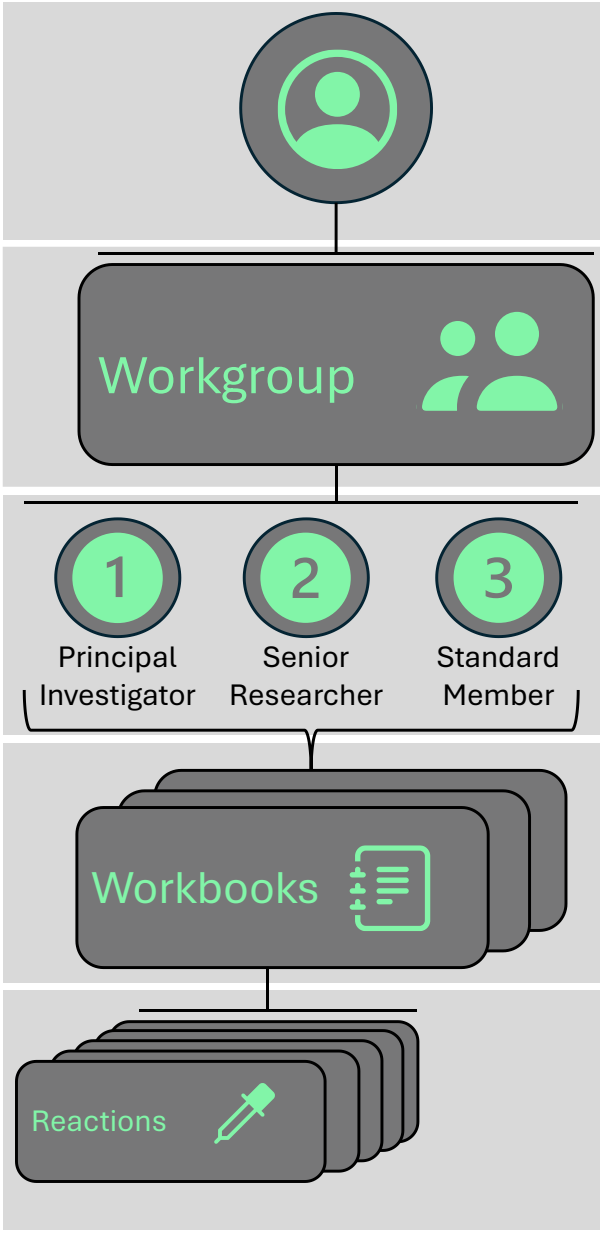
Key features include:

- Automatic calculations, hazard lookup and CAS database linkage
- Solvent selection guide
- Reaction summary including colour coding of solvent sustainability and hazards

For any queries please contact us at ai4green@nottingham.ac.uk.



AI4Green Work Structure



Users are researchers with accounts on AI4Green

Workgroups are collections of **Users**

Users have different levels of permission in **Workgroups**

Workbooks are collections of **Reactions** within **Workgroups**

Reactions contain experimental information obtained from the lab

Home Page

Home
This is the home page.

Demo
Try a limited version of the reaction constructor. No signup required.

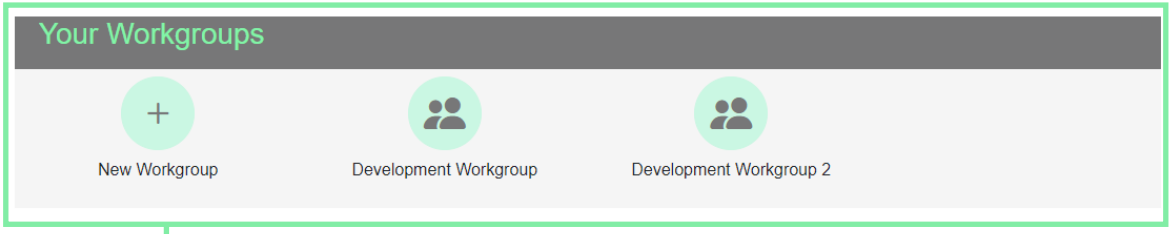
Solvents
Access our sustainable solvent selection tools

Retrosynthesis
Access our AI retrosynthesis tool

Workgroup
Access your Workgroups

Search
Search for a structure to retrieve all reactions where it is used.

Quick Access



Workgroups
You can create new Workgroups or access current Workgroups in the Quick Access Panel.

Workbooks
Selecting a Workgroup displays the Workbooks in that Workgroup

Reactions
Selecting a Workbook displays the Reactions in that Workbook

News Feed

No news items to show!

About AI4Green
More information about AI4Green

Help
Access our help guides and video tutorials.

User Dropdown
Modify your email/password, view notifications and customise sustainability colours

Create Workgroup

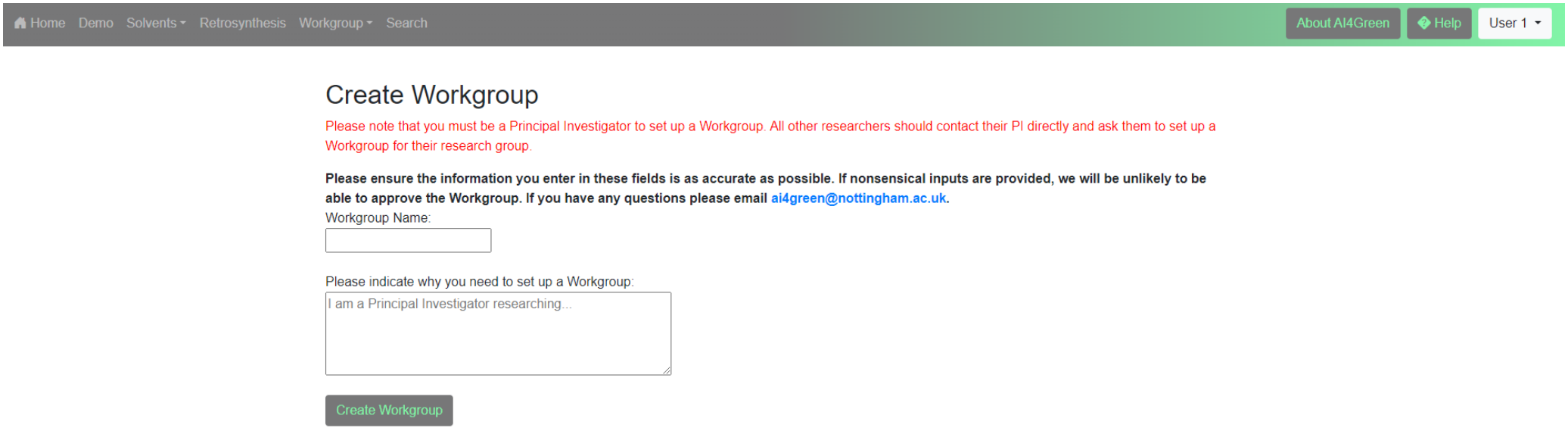
Create Workgroup

This is the create workgroup page. It can be accessed from the Quick Access panel on the home page or under the Workgroup tab of the navigation bar.

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.



Add Users to Workgroup

Manage Workgroup

Workgroups can be managed from the Manage Workgroup page. This can be accessed from the Workgroup tab in the navigation bar.

Users can also be removed from Workgroups under the Overview tab.

Add Users by Email

Principal Investigators can add users to a Workgroup using the email address registered to the Users AI4Green account.

The User will be sent a request which they must approve or deny before they are added to the Workgroup.

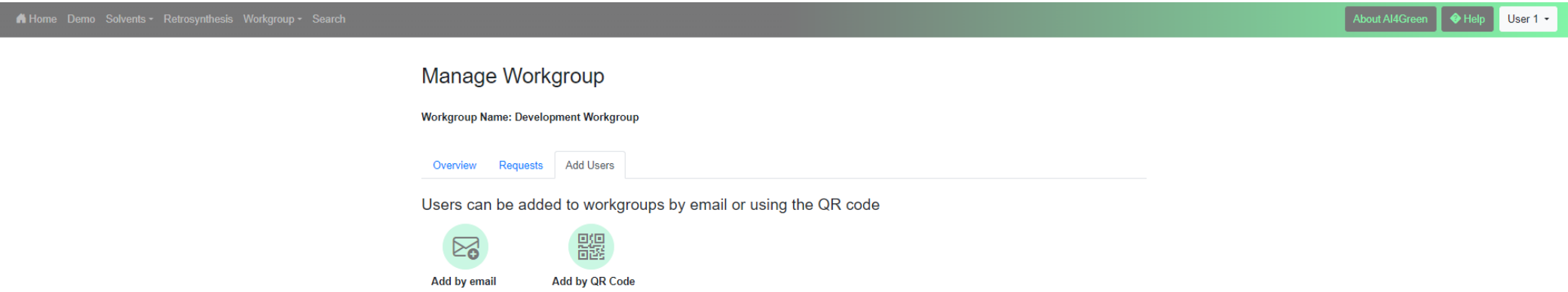
This is an easy way to add single Users to a Workgroup.

Add Users by QR Code

Principal Investigators can generate QR codes that allow users to join Workgroups. QR codes are valid for one year from the point of generation.

Scanning a QR code will send a request to the Principal Investigator, who must approve or deny the request before a user is added.

This is an easy way to add many Users to a Workgroup.



Create Workbook

Create Workbook

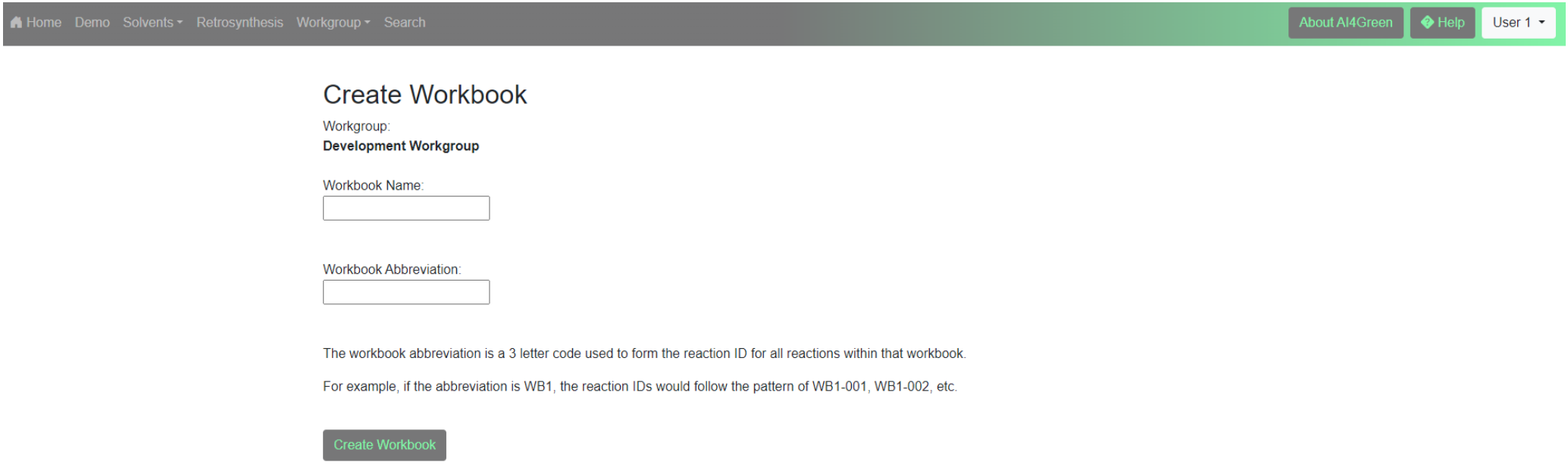
This is the create workbook page. It can be accessed from the Quick Access Panel on the home page or from the Workgroup tab in the navigation bar.

A workbook is designed to act as a collection of all researchers & reactions associated with a particular project. All Workbooks belong to a Workgroups, and 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 user type on the **manage workgroup** page.

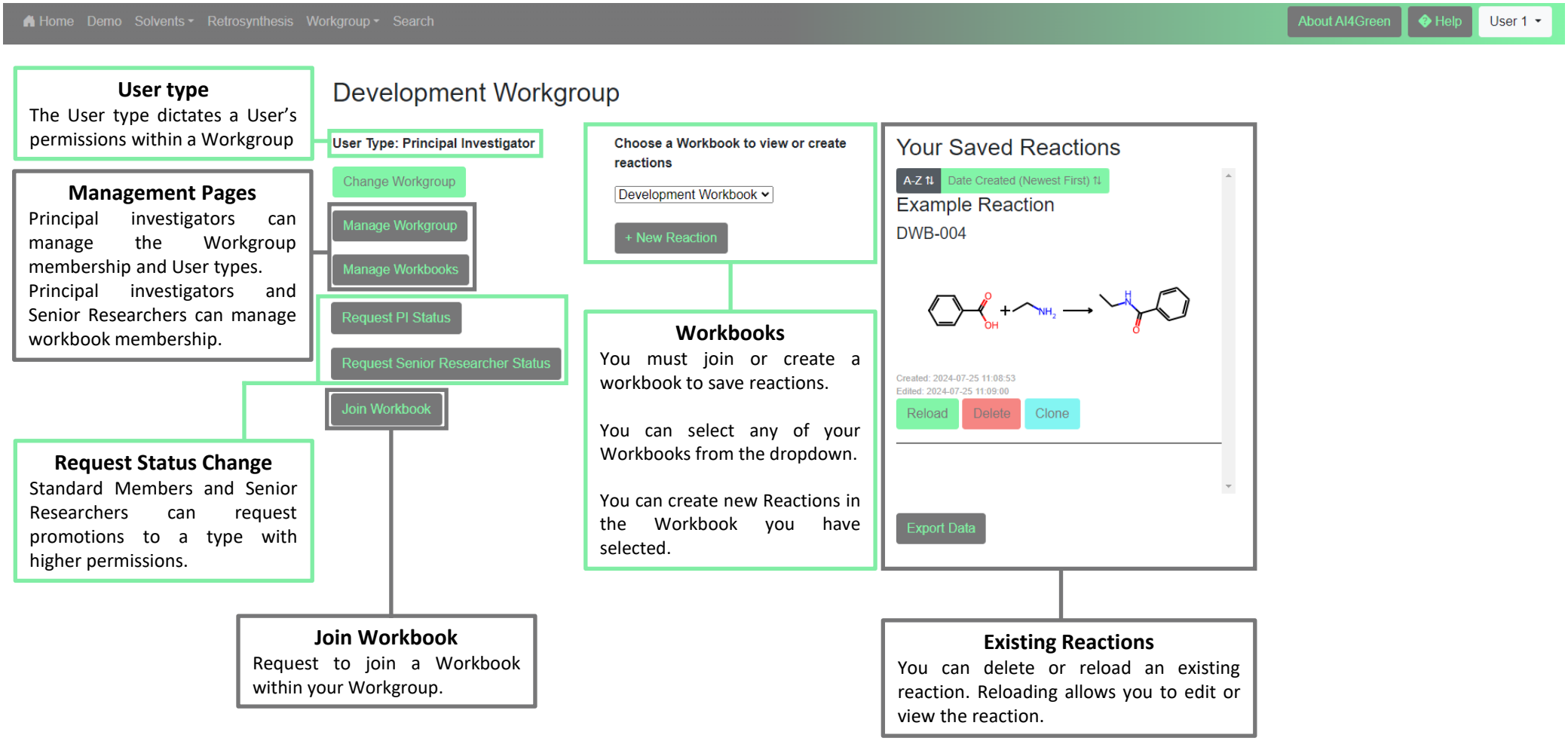
These actions can also be done by approving user requests.



Workgroup Page

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
The User type dictates a User's permissions within a Workgroup

Management Pages
Principal investigators can manage the Workgroup membership and User types. Principal investigators and Senior Researchers can manage workbook membership.

Request Status Change
Standard Members and Senior Researchers can request promotions to a type with higher permissions.

Join Workbook
Request to join a Workbook within your Workgroup.

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

You can select any of your Workbooks from the dropdown.

You can create new Reactions in the Workbook you have selected.

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.

Example Reaction

DWB-004

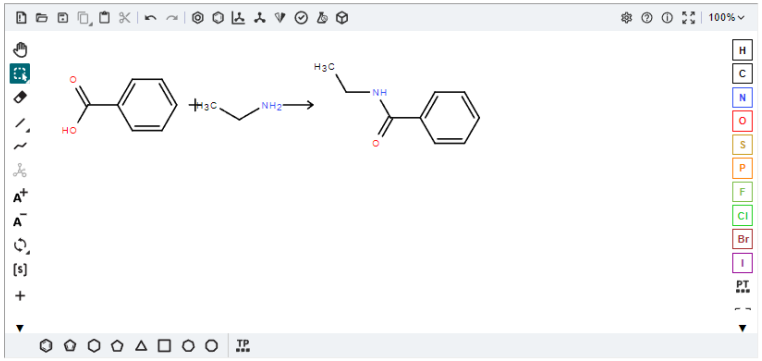
Need some help getting started?

Enter Tutorial Mode

Please sketch or upload your reaction to begin. Click here to view our Marvin JS help guide.

Please note compounds drawn above or underneath the arrow will not be recognised.

Selected Reaction Sketcher: MarvinJS ○ Ketcher ◉



Hint: You can copy & paste reaction schemes from ChemDraw by selecting the scheme and use CTRL + ALT + C to copy and then CTRL + V to paste into this sketcher

Example | Submit | Retrosynthesis

Example Reaction

Please describe your reaction

Please fill in the highlighted boxes to proceed

Reaction Class: Amide bond formation

№	Reactants	Limiting Reagent?	Mol.Wt	Density (g/mL)	Conc. (M)	Equiv.	Amount mmol	Volume mL	Mass mg	Physical Form	Hazards
1	Benzoic Acid	◉	122.12	-	-	1	-	-	-	-select-	H302-H315-H318-H319-H335-H372
2	Ethylamine	○	45.08	-	-	-	-	-	-	-select-	H220-H280-H302-H311-H314-H318-
	Catalysts/reagents Add new reagent to database										Add Reagent
	Solvents Add new solvent to database							mL			Add Solvent
	Product	**Desired Product?**					mmol		mg		
3	N-Ethylbenzamide	◉	149.19				-		-	-select-	H302

Summary

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.

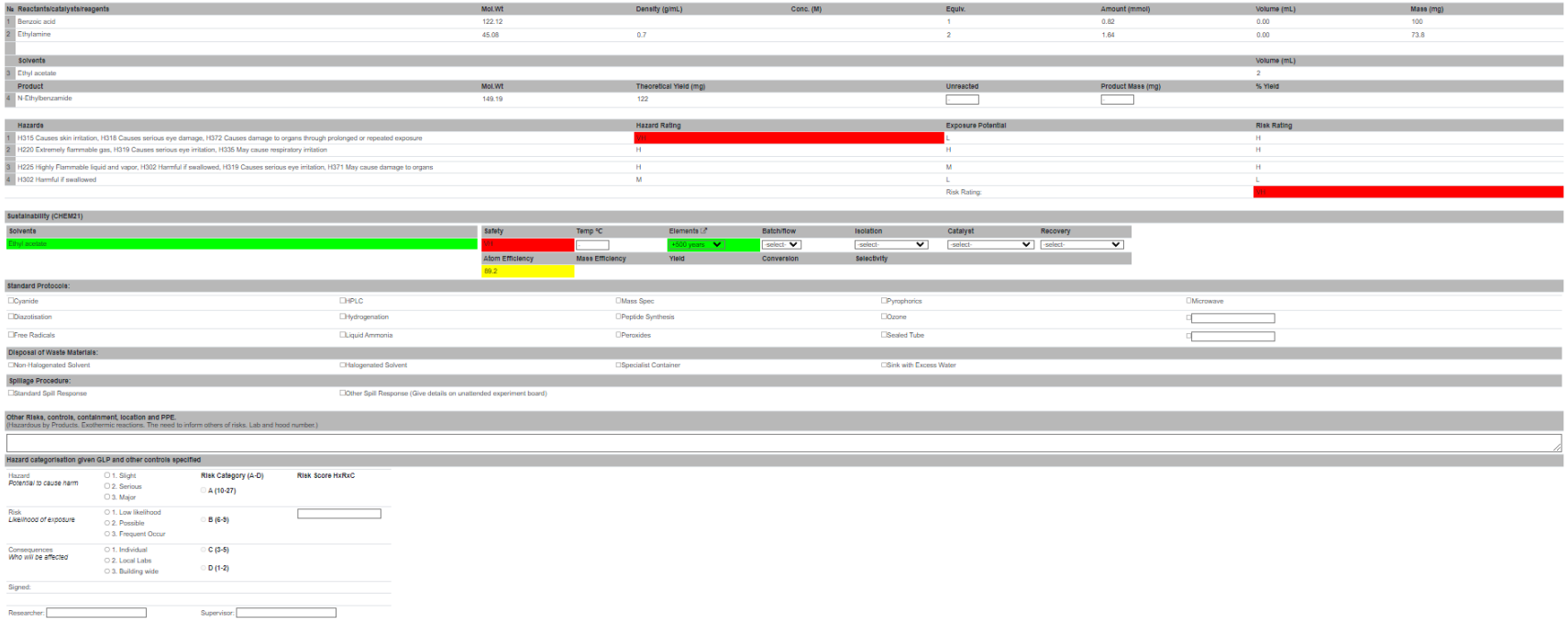
Autosave
All data entered into the reaction will be autosaved. Upon each successfully saved change, the message shown below will display in the top right of the screen.

Reaction Changes Saved | About AI4Green | Help | User 1

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**		
	69.2						

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

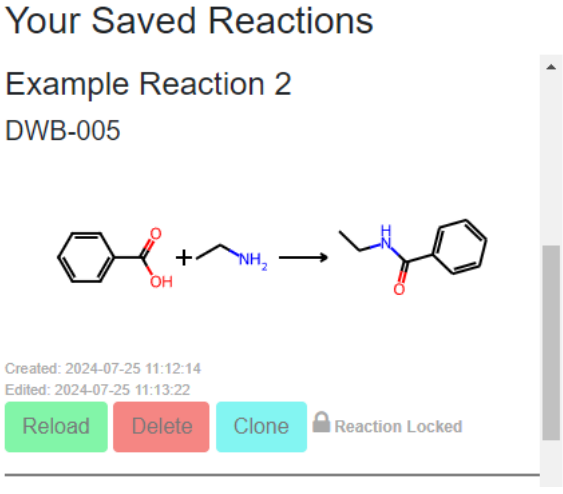
		Risk Category (A-D)	Risk Score HxRxC
Hazard *Potential to cause harm*	○ 1. Slight ○ 2. Serious ○ 3. Major	☐ A (10-27)	
Risk *Likelihood of exposure*	○ 1. Low likelihood ○ 2. Possible ○ 3. Frequent Occur	☐ B (6-9)	
Consequences *Who will be affected*	○ 1. Individual ○ 2. Local Labs ○ 3. Building wide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

Lock Reaction



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.