

### 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

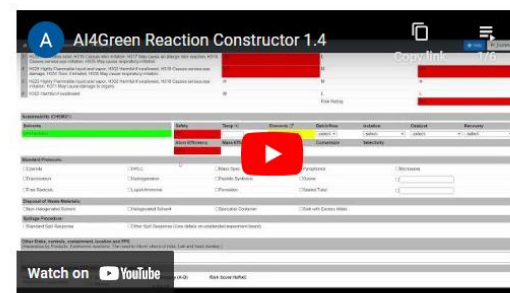
AI4Green provides an ELN including collaboration tools, data archival and management and green and sustainability metrics for organic chemistry.

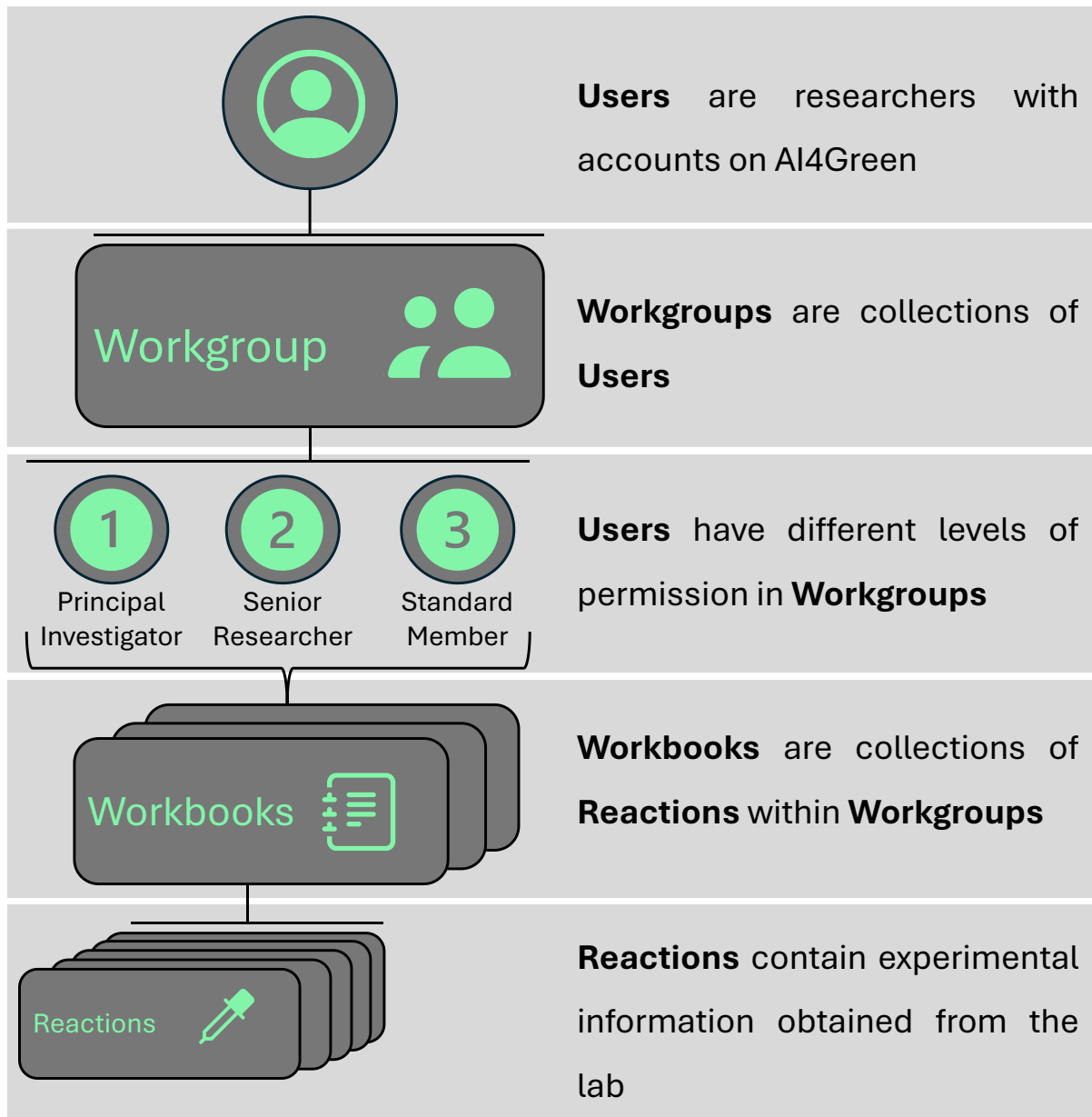
It is accessible via a web interface and fully available on an open source basis.

#### 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](mailto:ai4green@nottingham.ac.uk).





## 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.

Home Demo Solvents Retrosynthesis Workgroup Search

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User 1

Welcome to AI4Green, User 1!

## ☆ Quick Access

### Your Workgroups

+

New Workgroup



Development Workgroup



Development Workgroup 2

## 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

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.

## Create Workgroup

Please note that you must be a Principal Investigator to set up a Workgroup. All other researchers should contact their PI directly and ask them to set up a Workgroup for their research group.

Please ensure the information you enter in these fields is as accurate as possible. If nonsensical inputs are provided, we will be unlikely to be able to approve the Workgroup. If you have any questions please email [ai4green@nottingham.ac.uk](mailto:ai4green@nottingham.ac.uk).

Workgroup Name:

Please indicate why you need to set up a Workgroup:

Create 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 User's 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.

## Manage Workgroup

Workgroup Name: Development Workgroup

[Overview](#) [Requests](#) [Add Users](#)

Users can be added to workgroups by email or using the QR code



Add by email



Add by QR Code

## 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.

## Create Workbook

Workgroup:

**Development Workgroup**

Workbook Name:

Workbook Abbreviation:

The workbook abbreviation is a 3 letter code used to form the reaction ID for all reactions within that workbook.

For example, if the abbreviation is WB1, the reaction IDs would follow the pattern of WB1-001, WB1-002, etc.

Create Workbook

## 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.

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### 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.

## Development Workgroup

User Type: Principal Investigator

Change Workgroup

Manage Workgroup

Manage Workbooks

Request PI Status

Request Senior Researcher Status

Join Workbook

Choose a Workbook to view or create reactions

Development Workbook

+ New Reaction

### Workbooks

You must join or create a workbook to save reactions.

You can select any of your Workbooks from the dropdown.

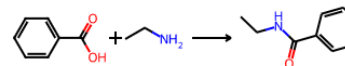
You can create new Reactions in the Workbook you have selected.

## Your Saved Reactions

A-Z | Date Created (Newest First)

### Example Reaction

DWB-004



Created: 2024-07-25 11:08:53

Edited: 2024-07-25 11:09:00

Reload

Delete

Clone

Export Data

### 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.

### Existing Reactions

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

## Example Reaction

DWB-004

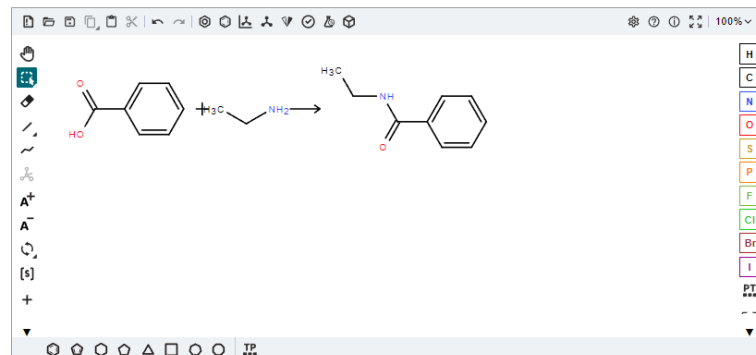
Need some help getting started?

[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:

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

[Summary](#)

## 1 Sketcher

Draw the reaction in here. Compounds drawn over the arrow will be ignored. Press "Submit" to continue.

## 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.

## 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.



### 3 Summary

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

No.	Reactants/catalysts/reagents	Mol. Wt.	Density (g/mL)	Conc. (M)	Equiv.	Amount (mmol)	Volume (mL)	Mass (mg)
1	Benzoic acid	122.12			1	0.62	0.00	100
2	Ethylamine	45.08	0.7		2	1.64	0.00	73.8

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

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	H	L	H
2. H220 Extremely flammable gas, H319 Causes serious eye irritation, H335 May cause respiratory irritation	H	M	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

Sustainability (CHEM21)	Safely	Temp. °C	Elements /#	Batch/flow	Isolation	Catalyst	Recovery
Atom Efficiency	99.2		100% green	select	select	select	select

**Standard Protocols:**

Cyanide       HPLC       Mass Spec       Pyrophorics       Microwave

Diazotization       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:**  
(Discipline by Product, Exothermic reactions, The need to inform others of risks, Lab and hood number.)

**Hazard categorisation given GLP and other controls specified**

Hazard Potential to cause harm:  1. Slight     2. Serious     3. Major      Risk Category (A-C):  A (10-27)     B (6-9)     C (3-5)     D (1-2)

Risk Likelihood of exposure:  1. Low likelihood     2. Possible     3. Frequent Occur

Consequences Who will be affected:  1. Individual     2. Local Lots     3. Building wide

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.

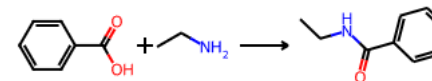
Lock Reaction



### Your Saved Reactions

#### Example Reaction 2

DWB-005



Created: 2024-07-25 11:12:14

Edited: 2024-07-25 11:13:22

Reload Delete Clone Reaction Locked

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.

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User 1 ▾

Welcome to AI4Green, User 1!

## ☆ Quick Access

### Your Workgroups

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New Workgroup



Development Workgroup



Development Workgroup 2

## ☆ News Feed

No news items to show!