

Accessing AI4Green

Web Browser

We recommend using Google Chrome.

URL

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



Please log in to access this page.

Sign In

☐ Remember Me

[Sign In](#)

New User? [Click to Register!](#)

Forgotten Your Password? [Click to Reset!](#)

Existing User

Sign in using your login credentials.

New User

Complete the registration form to create an account.

Getting Started

Home

This is the home page.

Demo

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

Solvent Guide

Access our sustainable Solvent Guide.

Workgroup

Quick access a Workgroup.

Search

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

[Home](#)
[Demo](#)
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[About AI4Green](#)
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JoeD

Welcome to AI4Green, JoeD!

AI4Green is an Electronic Laboratory Notebook built around encouraging green and sustainable chemistry.

[Learn more »](#)
[Quickstart Guide »](#)

Please select a Workgroup to get started

-Select Workgroup-

[Proceed to Workgroup](#)

[+ Join Existing Workgroup](#)

[+ Create Workgroup](#)

[Workgroup Membership Summary](#)

News Feed

The Solvent Surfer (Beta) is here!

- View reaction-specific PCA of solvent space
- Up to 16 physicochemical solvent descriptors
- Interact and shape embeddings with Interactive Mode
- Access through Solvent Guide or during reaction setup

[Click here to get started!](#)
[Click here for help!](#)

2024-01-31 12:07:36

AI4Green User Feedback

Please use the below form to provide feedback on your initial impressions or experiences using AI4Green.

[Feedback Form](#)

[Hazard Disclaimer](#) |
 [Privacy Notice](#) |
 [Twitter](#) |
 [GitHub](#)

Hazard data sourced from ECHA references on PubChem

Help

Access our help guides and video tutorials.

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.

Manage Account

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

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.

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.

Workgroup Name:

Please indicate why you need to set up a Workgroup:

I am a Principal Investigator researching...

Create Workgroup

Create Workbook

Workgroup:

The Sam Group

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

Getting Started – Standard users

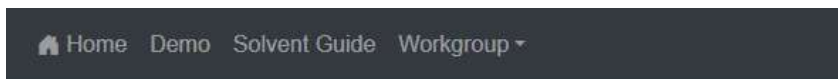
1 Join workgroup

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.



Request to Join a Workgroup

Development-Workgroup ▼

Request to Join Workgroup

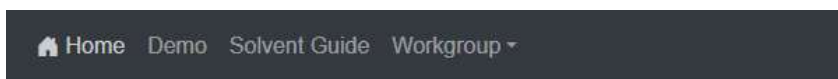
2 Join workbook

This is the join workbook page

Once you are 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.



Request to Join a Workbook

New Project ▼

Request to Join Workbook

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.

[Home](#)
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[SamB ▾](#)

The Sam Group

Workgroup Pending Moderation

User Type: Principal Investigator

[Change Workgroup](#)
[Manage Workgroup](#)
[Manage Workbooks](#)
[Request PI Status](#)
[Request Senior Researcher Status](#)
[Join Workbook](#)

Workbooks

You must join or create a workbook to save reactions.

Choose a Workbook to view or create reactions

New Project ▾

[+ New Reaction](#)

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.

Your Saved Reactions

A-Z 🔼
Date Created (Newest First) 🔼

Amide Coupling

NP1-001

2023-02-09 13:42:40 575523

[Reload](#)
[Delete](#)

Existing Reactions

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

Reactions

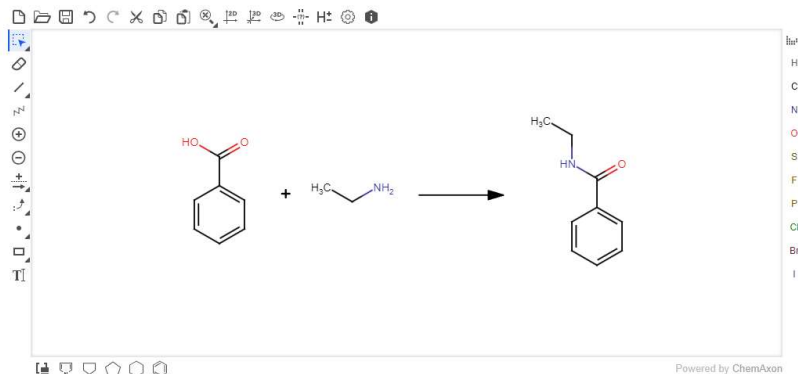
1 Sketcher

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

Reaction Builder

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.



Example

Submit

Amide Coupling

Please describe your reaction

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.

Please fill in the highlighted boxes to proceed

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-"/>	H315-H318-H372
2	Ethylamine	<input type="radio"/>	45.08	-	-	<input type="text" value="-"/>	-	-	<input type="text" value="-"/>	<input type="text" value="-select-"/>	H220-H319-H335
Catalysts/reagents											<input type="button" value="Add Reagent"/>
Solvents											<input type="button" value="Add Solvent"/>
Product											
3	N-Ethylbenzamide	<input checked="" type="radio"/>	149.19	-	-	-	-	-	<input type="text" value="-select-"/>	<input type="text" value="H302"/>	

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

PI_Dummy

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.

No	Reactants/catalysts/reagents	Mol.Wt	Density (g/mL)	Conc. (M)	Equiv.	Amount (mmol)	Volume (mL)	Mass (mg)
1	Benzene acid	122.12			1	0.82	0.00	100
2	Ethylamine	45.08	0.7		2	1.64	0.00	73.6

Solvents							
3	Ethyl acetate						Volume (mL)
4	N-Ethylbenzamide	149.19	122				% Yield

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		L	H
2 H226 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

Sustainability (CHEM21)							
Solvents	Safety	Temp. °C	Elements (P)	Batch/Flow	Isolation	Catalyst	Recovery
Ethyl acetate	High		100% green	Batch	Control	Batch	Batch
	Atom Efficiency	Mass Efficiency	Yield	Conversion	Selectivity		
	88.2						

Standard Protocols:							
<input type="checkbox"/> Cyanide	<input type="checkbox"/> HPLC	<input type="checkbox"/> Mass Spec	<input type="checkbox"/> Pyrophorics	<input type="checkbox"/> Microwave			
<input type="checkbox"/> Diazotisation	<input type="checkbox"/> Hydrogenation	<input type="checkbox"/> Peptide Synthesis	<input type="checkbox"/> X-ray	<input type="checkbox"/> Sealed Tube			
<input type="checkbox"/> Free Radicals	<input type="checkbox"/> Liquid Ammonia	<input type="checkbox"/> Peroxides					

Disposal of Waste Materials:			
<input type="checkbox"/> Non-Halogenated Solvent	<input type="checkbox"/> Halogenated Solvent	<input type="checkbox"/> Specialist Container	<input type="checkbox"/> Sink with Excess Water

Spillage Procedure:	
<input type="checkbox"/> Standard Spill Response	<input type="checkbox"/> Other Spill Response (Give details on unattended experiment board)

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

Hazard categorisation given GHS and other controls specified			
Hazard Potential to cause harm	<input type="radio"/> 1. Slight <input type="radio"/> 2. Serious <input type="radio"/> 3. Major	Risk Category (A-D)	Risk Score HSE/C
		<input type="radio"/> A (10-27)	
Risk Likelihood of exposure	<input type="radio"/> 1. Low likelihood <input type="radio"/> 2. Possible <input type="radio"/> 3. Frequent Occur	<input type="radio"/> B (6-9)	
Consequences Who will be affected	<input type="radio"/> 1. Individual <input type="radio"/> 2. Local Lab <input type="radio"/> 3. Building wide	<input type="radio"/> C (3-5) <input type="radio"/> D (1-2)	
Signed:			
Researcher: <input type="text"/>	Supervisor: <input type="text"/>		

4 Locking

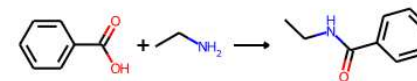
Once the reaction is complete and you do not wish to make more changes, click the "Lock Reaction" button. The reaction is now locked for editing but can still be viewed.

Lock Reaction

Your Saved Reactions

A-Z 11 Date Created (Newest First) 11

Amide coupling



2022-08-24 16:59:32.771034

Reload

Delete

Reaction Locked

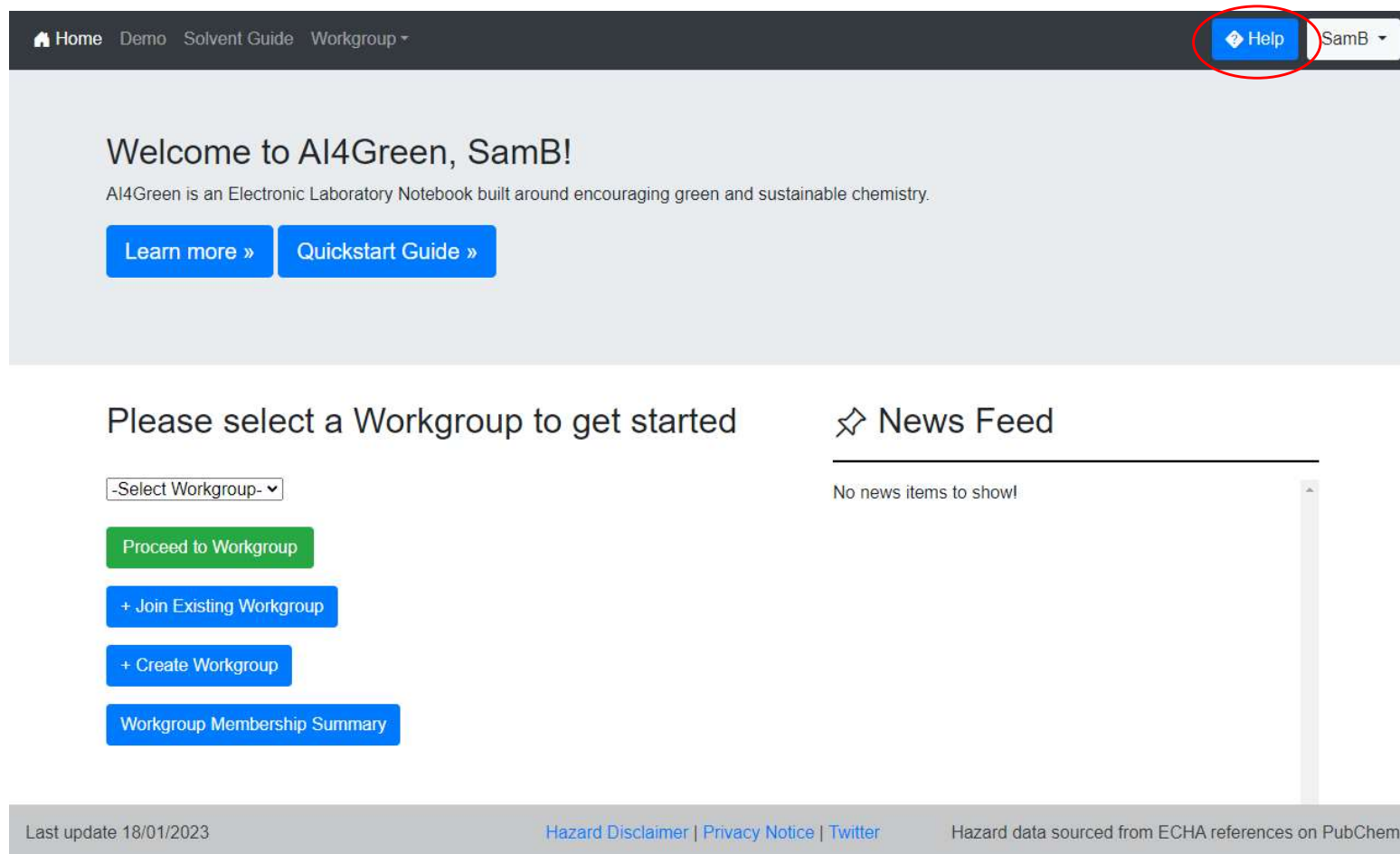
Additional Information

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.



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Help SamB ▾

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[Workgroup Membership Summary](#)

News Feed

No news items to show!

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