

AI₄Green

Version 1.6 User Guide

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of Engineering

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1. Introduction

AI4Green is an electronic laboratory notebook (ELN) that uses artificial intelligence to encourage green and sustainable chemistry. It is developed by the [Hirst Group](#) at the University of Nottingham and is completely open access and free to use.

AI4Green includes all the features you need for carrying out experimental chemistry, from drawing chemical structures to automatically finding and providing their associated hazard data. The AI4Green reaction constructor streamlines reaction design, provides a cloud-based back-up for all experimental data and automatically calculates green metrics to highlight the sustainability of each reaction. This shows you how green and sustainable your chemistry is and highlights the areas that should be targeted to reduce environmental impact.

Greener choices are also identified using cutting-edge artificial intelligence tools that are integrated directly into AI4Green. These tools can aid in the identification of greener solvent alternatives (Solvent Surfer) or green retrosynthetic pathways (Retrosynthesis). Tools for assessing life cycle analysis and carrying out design of experiments are in development and will be released in future versions.

Though AI4Green has been designed for traditional synthetic organic chemistry, support for high-throughput experimentation and polymer chemistry is currently being developed and will be released in future versions.

Note that hazard data was sourced from ECHA references on PubChem.

Details of our hazard disclaimer can be found here:

https://ai4green.app/auth/hazard_disclaimer

Details of our privacy notice can be found here:

https://ai4green.app/auth/privacy_notice

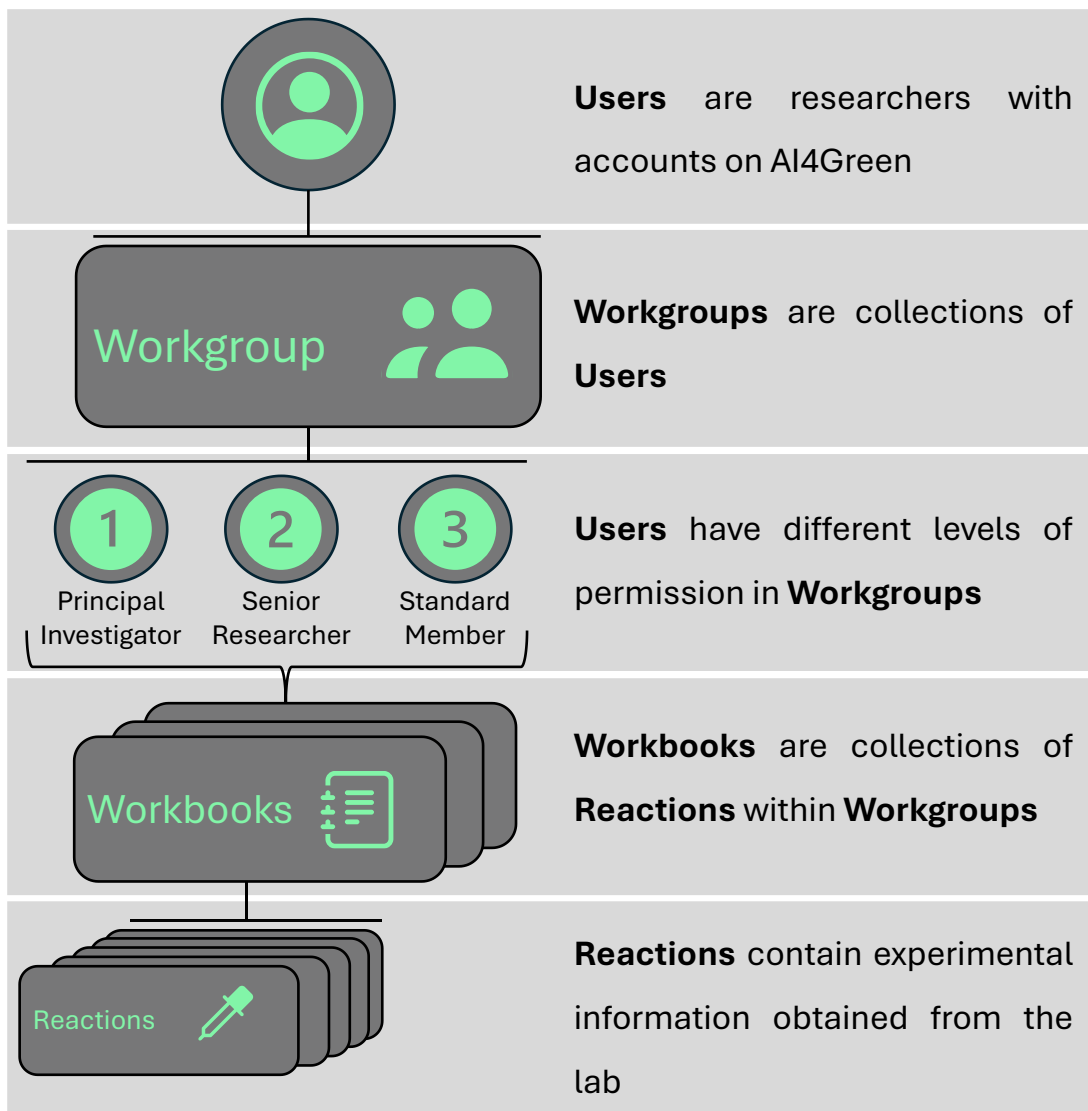
2. AI4Green Work Structure

Users in AI4Green are organised into [Workgroups](#). These are collections of users that work in a similar area, such as users with the same supervisor or users working on related projects.

Within [Workgroups](#) there are [Workbooks](#). These are smaller collections of users who are working on the same project, where it makes sense to group their work together. Alternatively, users may prefer to each have their own [Workbook](#) within a [Workgroup](#). A [Workbook](#) belongs to a [Workgroup](#), and all members of the [Workbook](#) must also belong to that [Workgroup](#).

Within [Workbooks](#), [Reactions](#) can be created. These are individual entries that relate to chemical reactions you might conduct in the laboratory. This is where your experimental data is stored.

This simple schematic represents the work structure of AI4Green. Organising users in this way allows collaboration within [Workgroups](#).



3. Getting Started

A Quick Start Guide is available from our help page: <https://ai4green.app/info>

AI4Green can be accessed at <https://ai4green.app/> from any web browser, but we highly recommend using Google Chrome.

The landing page will prompt you to log in or register if you do not have an account. Our YouTube channel provides some excellent quick start videos, which can be accessed from this page.

Home Demo About AI4Green Help Log in

AI₄Green

Username

Password

Sign In

Remember Me

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

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

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 Reaction Constructor 1.4

Watch on [YouTube](#)

AI Green

Hazard Disclaimer | Privacy Notice | Twitter | GitHub

Hazard data sourced from ECHA references on PubChem

3.1. Registering as a New User

The first step to using the AI4Green webapp is creating an account. This allows you to access the full range of features in AI4Green. If you want to try out the Reaction Constructor before registering for an account, you can do so by clicking the [Demo](#) quick link on the [Navigation bar](#).

[Click to Register!](#) will direct you to the registration page, which will prompt you to enter a username, your full name, email address and a unique password. Please note that only letters, numbers and underscores are permitted in your username. You will also have to agree to our [privacy policy](#) and [hazard disclaimer](#), please make sure you read these before registering!

Register

Username (Only letters, numbers, and underscores)

Username

Fullname

Full Name

Email

Email

Password

Password

Confirm Password

Repeat Password

I have read and agree to the conditions in the [privacy notice](#)

I have read and agree to the conditions in the [hazard disclaimer](#)

I'm not a robot

reCAPTCHA

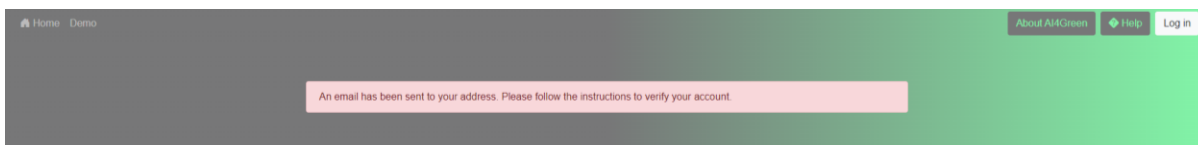
Register

AI₄Green

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

Hazard data sourced from ECHA references on PubChem

You will have to verify your email address before you can access all the features of AI4Green. Emails typically take between two and five minutes to come through. If you have not received an email, try checking your spam folder.



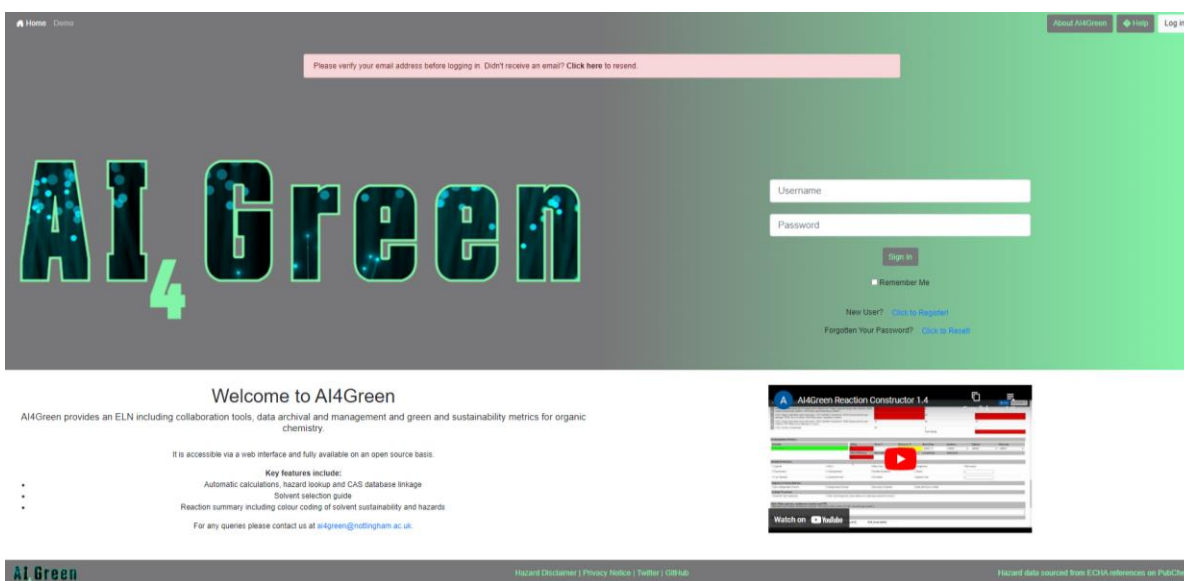
Sign In

 Remember Me

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

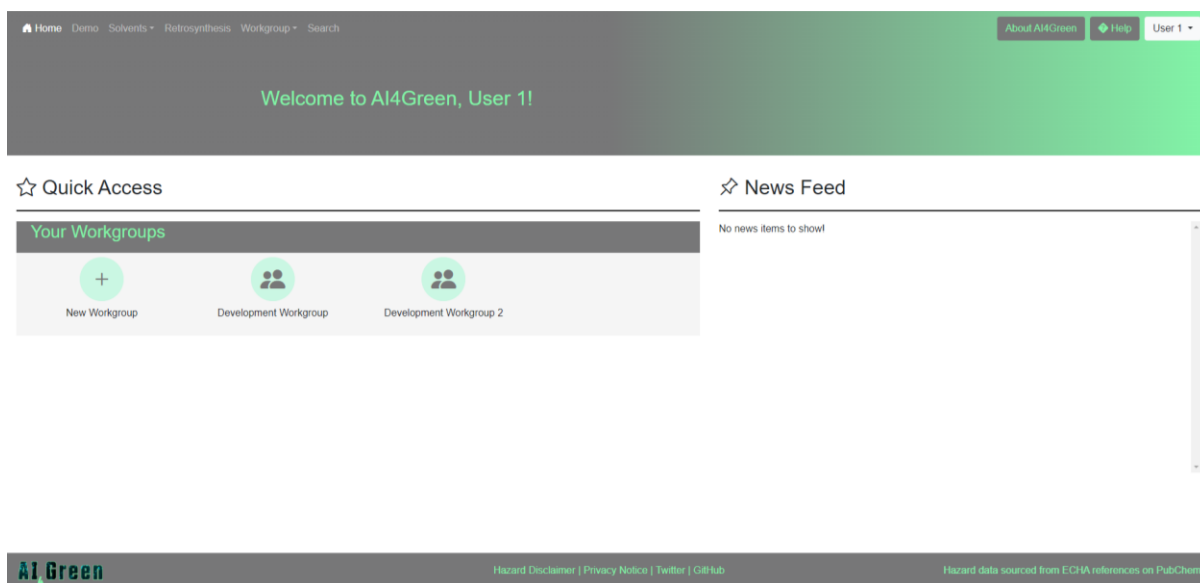
Forgotten Your Password? [Click to Reset!](#)

Attempting to login before verifying your email address will redirect you to the landing page. From here, you can request to send the verification email again.



3.2. The Home Page

After logging in, you are taken to the home page. From this page you can access all the features in AI₄Green. The News Feed displays any messages for the AI₄Green community. The Quick Access panel gives a summary of your [workgroups](#), [workbooks](#), and [reactions](#). The structures of workgroups and workbooks are described later in this guide.



New Workgroups can be created by clicking on the “New Workgroup” icon which will take you to the [New Workgroup](#) page. Selecting the Workgroup icon “Development Workgroup” generates a new panel that shows the Workbooks included in this Workgroup.

The screenshot shows the AI4Green user interface. At the top, there is a navigation bar with links for Home, Demo, Solvents, Retrosynthesis, Workgroup, and Search. On the right, there are buttons for About AI4Green, Help, and a user profile for User 1. Below the navigation bar, a green banner displays "Welcome to AI4Green, User 1!". The main content area is divided into two columns. The left column, titled "Quick Access", contains two sections: "Your Workgroups" and "Workbooks in Development Workgroup". "Your Workgroups" includes a "New Workgroup" icon (a plus sign) and two "Development Workgroup" icons (each with a plus sign and a group of people icon). "Workbooks in Development Workgroup" includes a "New Workbook" icon (a plus sign) and a "Development Workbook" icon (a document with a plus sign). The right column, titled "News Feed", shows "No news items to show". At the bottom of the page, there is a footer with the AI4Green logo, links for Hazard Disclaimer, Privacy Notice, Twitter, and GitHub, and a note that hazard data is sourced from ECHA references on PubChem.

New workbooks can be created by clicking on the “New Workbook” icon which will take you to the [New Workbook](#) page. Only Workgroup owners can create new Workbooks within Workgroups. If you do not have permissions to create new Workbooks, you will be redirected to the home page. Selecting the icon “Development Workbook” generates a new panel that shows the Reactions contained in this Workbook.

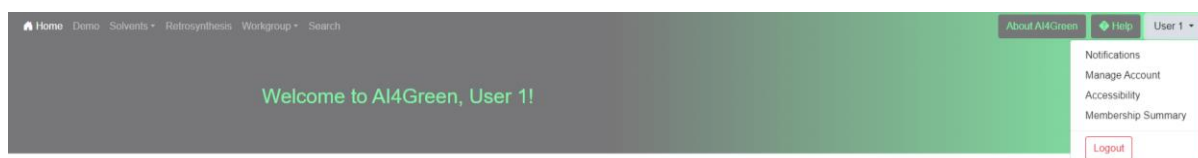
This screenshot is similar to the first one, showing the AI4Green user interface. The layout is the same, but the "Quick Access" section now includes a third section: "Recent Reactions in Development Workbook". This section contains a "New Reaction" icon (a plus sign) and two reaction icons labeled "DWB-002" and "DWB-001", each with a pipette icon. The "News Feed" section remains empty with "No news items to show". The footer is identical to the first screenshot.

Any member of a Workbook can create a reaction with the “New Reaction” icon. Selecting any Reaction icon loads the corresponding [Reaction](#) page.

3.3. The Navigation Bar

The top navigation bar is the same on any page in AI4Green, and the left-hand side provides quick links to the [home page](#), [demo reaction constructor](#), [Solvent Guide](#) or [Solvent Surfer](#) (under the Solvents Tab), [Retrosynthesis tool](#), [Workgroup Management](#) page (under Workgroups tab) and the [Search](#) function.

On the right-hand side, you can learn more about AI4Green by following the “About AI4Green” quick link or get more [help](#) by following the “Help” quick link. The user drop down allows you to manage your account by viewing [notifications](#), [change your email or password](#), [edit hazard colours](#) and see a [summary of your Workgroup and Workbook memberships](#).



3.3.1. Search

The Navigation bar provides a quick link to the Search page. From this page, you can search your [Workgroups](#) and [Workbooks](#) for specific chemical structures and find exactly which [Reactions](#) contain them. The search can be limited to specific Workgroups and Workbooks, or you can search though all that you are a member of.

3.3.2. Notifications

Your notifications are accessible from the User dropdown menu on the right-hand side of the [Navigation bar](#). These are used to keep you up to date with any requests you have made. These include being added to a Workgroup or Workbook, changing user status or exporting data. You will receive an email when you have notifications pending on AI4Green.

Home Demo Solvents Retrosynthesis Workgroup Search About AI4Green Help Standard User

Notifications

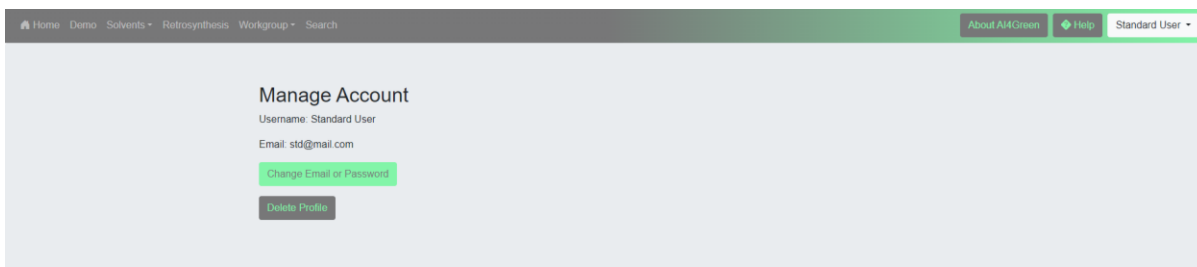
Request to become a Senior Researcher
Your request to become a Senior Researcher in Workgroup, Development Workgroup, has been approved!
2024-07-24 15:19:16.006846

Your Request to join Development Workgroup
Your request to join Workgroup, Development Workgroup has been denied.
2024-07-24 14:50:29.706804

AI Green Hazard Disclaimer | Privacy Notice | Twitter | GitHub Hazard data sourced from ECHA references on PubChem

3.3.3. Manage Account

You can manage your account from the User dropdown on the right-hand side of the [Navigation bar](#). This lets you change your email, change your password, or delete your account.



3.3.4. Accessibility

You can choose which colours represent which hazards on the accessibility page. This page is easily accessible from the User dropdown on the right-hand side of the [Navigation bar](#). The colours you select will be replicated across AI4Green. You can restore the default colours at any time. Make sure to save your changes before exiting this page.

Accessibility Hazard Colours

AI4Green uses four colours to denote different hazard levels.

Recommended	
The least hazardous classification. Attention should still be taken to specific hazards (e.g. hazard codes) and safety/disposal procedures.	
Fill Colour	<input type="text" value="Green"/>
Text Colour	<input type="text" value="Black"/>
Preview	Recommended

Problematic	
Caution should be taken with this classification. Care should be taken to follow health, safety, and environmental procedures.	
Fill Colour	<input type="text" value="Yellow"/>
Text Colour	<input type="text" value="Black"/>
Preview	Problematic

Hazardous	
These procedures should be avoided, but may still be acceptable in certain circumstances. Extreme care should be taken to mitigate hazards.	
Fill Colour	<input type="text" value="Red"/>
Text Colour	<input type="text" value="Black"/>
Preview	Hazardous

Highly Hazardous	
Solvents only: this classification indicates banned or highly problematic solvents, the use of which should be highly discouraged.	
Fill Colour	<input type="text" value="Dark Red"/>
Text Colour	<input type="text" value="White"/>
Preview	Highly Hazardous

3.3.5. Membership summary

A summary of your Workgroup and Workbook memberships can be accessed from the User dropdown on the right-hand side of the [Navigation bar](#). You can select a Workgroup that you are a part of and search which Workbooks you are a member of.

Workgroup Membership Summary

Workgroups:

Development Workgroup

Find Workbooks

No workgroups shown? Click [here](#) to create a workgroup.

Workgroup Selected:

Development Workgroup

You are a member of the following workbooks within this workgroup:

Development-Workbook-1

Development Workbook

4. Workgroups

A Workgroup is a group of users that can collaborate on various projects. A Workgroup contains [Workbooks](#) that contain [Reactions](#), and users within a Workgroup can be added to different [Workbooks](#) to view those contained [Reactions](#).

4.1. User types

There are three different user types with different permissions. All users can create, construct and save Reactions.

4.1.1. Principal Investigator

The top level of authorisation. When a user creates a Workgroup, they will become the principal investigator of that Workgroup. Principal investigators can add/remove users from the Workgroup and change their user types via the [Manage Workgroup page](#). They can create new Workbooks and add/remove users from workbooks via the Manage Workbooks page.

In a Workgroup, it's possible to have multiple principal investigators. We recommend adding at least one additional trusted user as a principal investigator. This ensures efficient management of administrative tasks for the Workgroup.

4.1.2. Senior Researcher

Senior Researchers can create new workbooks and add/remove users from workbooks via the [Manage Workbooks page](#), however they cannot access the [Manage Workgroup page](#). Senior Researchers can submit a request to the Principal Investigator to be promoted to a Principal Investigator from the [Workgroup page](#).

4.1.3. Standard Member

Standard Members can construct and save reactions, but they cannot create new workbooks or add/remove other users. Standard Members can submit a request to the Principal Investigator to be promoted to Senior Researcher from the [Workgroup page](#).

Permission	Principal Investigator	Senior Researcher	Standard Member
Manage Workgroup Access	✓	✗	✗
Change User Types	✓	✗	✗
Manage Workbook Access	✓	✓	✗
Create New Workbooks	✓	✓	✗
Create Reactions	✓	✓	✓
Request Status Change	✗	✓	✓

4.2. Creating Workgroups

Workgroups can be created by clicking on the “New Workgroup” icon in the Quick Access panel on the [home page](#). This navigates you to the “Create Workgroup” page, which prompts you to enter a name for your Workgroup and a brief explanation of your research. Each Workgroup must be approved by our admin team, so if nonsensical inputs are provided your Workgroup will not be approved.

The screenshot shows the 'Create Workgroup' page in the AI₄Green system. At the top, there is a navigation bar with links for Home, Demo, Solvents, Retrosynthesis, Workgroup, and Search. On the right side of the navigation bar, there are buttons for 'About AI₄Green', 'Help', and 'User 1'. The main content area is titled 'Create Workgroup' and contains the following text: '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.' Below this, a note states: '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.' There are two input fields: 'Workgroup Name' and a larger text area for 'Please indicate why you need to set up a Workgroup'. The text area contains the text 'I am a Principal Investigator researching...'. At the bottom of the form is a 'Create Workgroup' button. The footer of the page includes the AI₄Green logo, links for 'Hazard Disclaimer | Privacy Notice | Twitter | GitHub', and a note: 'Hazard data sourced from ECHA references on PubChem.'

4.3. The Workgroup Page

Once your Workgroup has been created and approved, you will be able to access your Workgroup from the Workgroup dropdown in the [navigation bar](#). Selecting your Workgroup from this dropdown takes you to the Workgroup page, which shows the user's type, a dropdown with the workbooks they belong to and a scrollable list of the [saved Reactions](#) in that workbook. These Reactions can be [exported](#) to both human-readable and machine-readable formats by clicking the "Export" button.

Depending on the user type, different options are visible. Senior Researchers and Principal Investigators can access [Manage Workbooks](#) and only Principal Investigators can access [Manage Workgroups](#). Clicking on either of these buttons takes you to the corresponding page.

The screenshot shows the 'Development Workgroup' page. At the top, there is a navigation bar with links for Home, Demo, Solvents, Retrosynthesis, Workgroup, and Search. On the right side of the navigation bar, there are links for 'About AI4Green', 'Help', and 'User 1'. The main content area is titled 'Development Workgroup' and is divided into three sections:

- User Type: Principal Investigator**: This section contains three buttons: 'Change Workgroup' (highlighted in green), 'Manage Workgroup', and 'Manage Workbooks'.
- Choose a Workbook to view or create reactions**: This section features a dropdown menu currently set to 'Development Workbook' and a '+ New Reaction' button.
- Your Saved Reactions**: This section is a large, empty scrollable area with a vertical scrollbar on the right. Below this area is an 'Export Data' button.

At the bottom of the page, there is a footer with the AI4Green logo, a 'Hazard Disclaimer | Privacy Notice | Twitter | GitHub' link, and a note that 'Hazard data sourced from ECHA references on PubChem'.

From this page, Senior Researchers and Standard Members can request a change of status. See below for an example for a Standard Member. Senior Researchers and Standard Members can also request to [join a Workbook](#) in the Workgroup using the "Join Workgroup" button.

Development Workgroup

User Type: Standard Member

Change Workgroup

Request PI Status

Request Senior Researcher Status

Join Workbook

Choose a Workbook to view or create reactions

No Workbooks to Show

4.4. Managing Workgroups

4.4.1. Overview

The Workgroup Management page is accessible from the [Workgroup page](#) and is only allowed for Principal Investigators. From here Principal Investigators can see which users are members of their Workgroup and their current membership level. This can be changed at any time by using the action buttons, which promote, demote or remove users from the Workgroup.

Manage Workgroup

Workgroup Name: Development Workgroup

Overview			Requests	Add Users
Name	Email	Actions		
Principal Investigators				
User 1	user@mail.com		↓ PI to SR	Remove from Workgroup
Senior Researchers				
user 2	user2@mail.com	↑ SR to PI	↓ SR to SM	Remove from Workgroup
Standard Members				
Standard User	std@mail.com	↑ SM to SR		Remove from Workgroup

4.4.2. Requests

Any requests from users for a change of status or to be added to the Workgroup will be shown under the Requests tab. The Principal Investigator can then approve or deny requests.

The screenshot shows the 'Manage Workgroup' page for 'Development Workgroup'. The 'Requests' tab is active, displaying a table with the following data:

Name	Email	Current Role	New Role	Time	Decision
Standard User	std@mail.com	Standard Member	Senior Researcher	2024-07-24 13:35:21	Approve Deny

4.4.3. Add Users

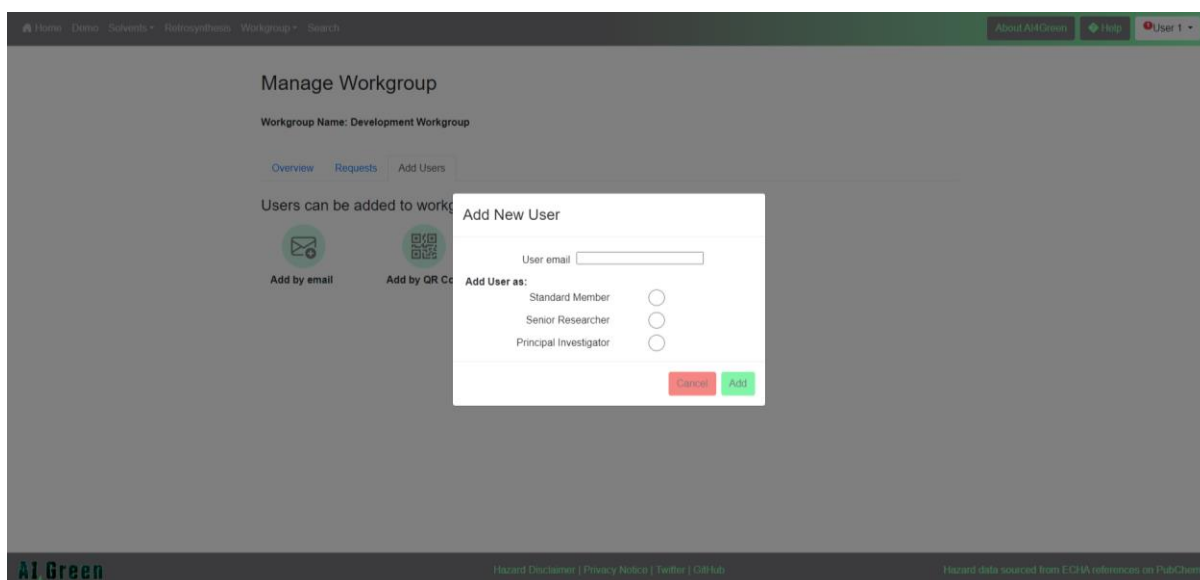
Adding users to Workgroups has changed from previous versions. There are now two ways to add users to a Workgroup, via email or QR code.

The screenshot shows the 'Manage Workgroup' page for 'Development Workgroup'. The 'Add Users' tab is active, displaying the following options:

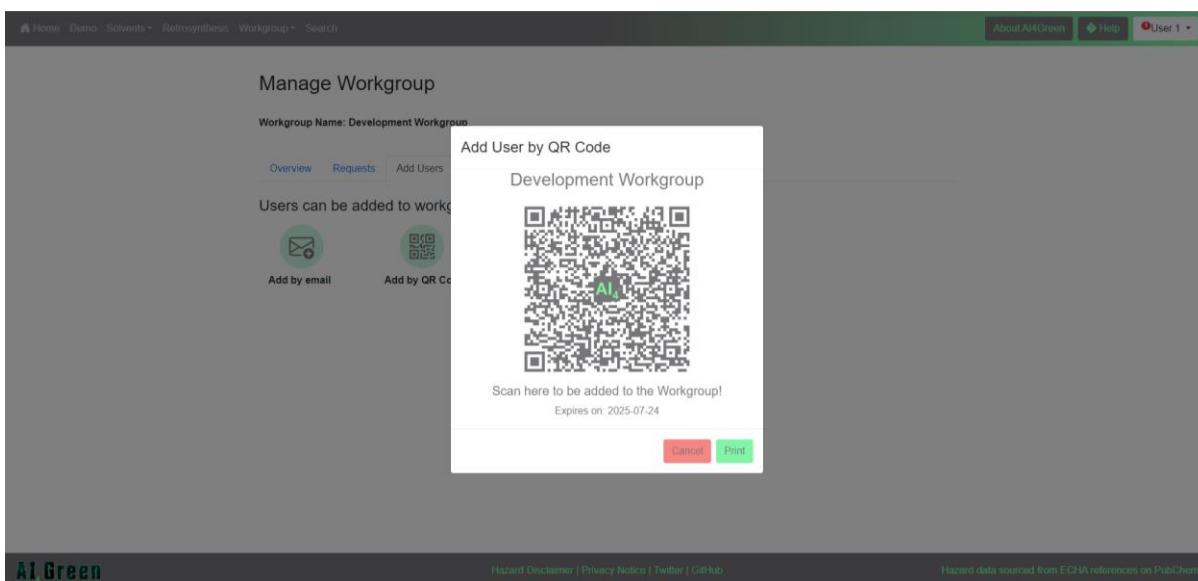
Users can be added to workgroups by email or using the QR code

- Add by email
- Add by QR Code

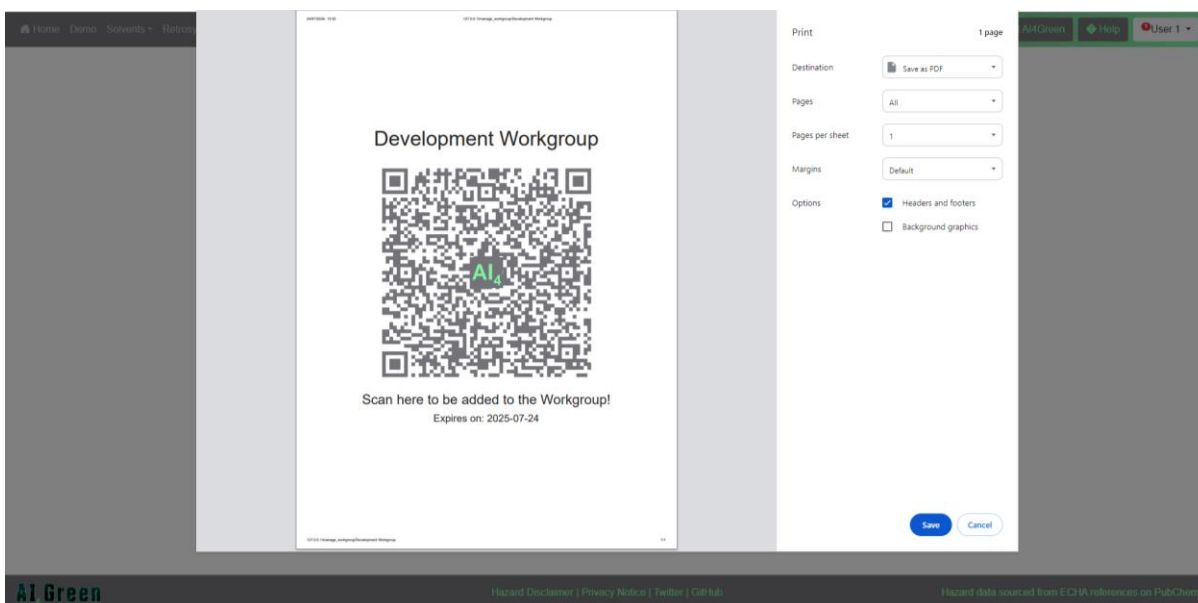
Principal Investigators can add users by their registered AI4Green email address by clicking on the “Add by email” icon. This will prompt you to enter the email address of the user you want to add and to select a membership level for the new user. This will [send a request](#) to the added user and will need their approval before they are added. This provides an extra layer of security.



Alternatively, users can be added by scanning a generated Workgroup QR code. This provides an alternative option and allows for the addition of multiple users without having to enter each individual email, which can be time consuming. Instead, QR codes can be circulated to users who would like to join your Workgroup. The QR codes can be generated by selecting the “Add by QR Code” icon. The generated QR code is valid for one year and the expiration date is clearly displayed.



Click the “Print” button will allow to either print or save your QR code, which can then be sent to the users you would like to add.



When a user scans a QR code, a membership request is sent to the Principal Investigator of the Workgroup and their approval is needed before the user is added. This provides an extra layer of security. You will receive a [Notification](#) about this request, which you can then view under the [request](#) tab.

Manage Workgroup

Workgroup Name: Development Workgroup

Overview Requests Add Users

Name	Email	Current Role	New Role	Time	Decision
Standard User	std@mail.com	Standard Member	Senior Researcher	2024-07-24 13:35:21	Approve Deny

4.5. Joining Workgroups

Users can only be added to Workgroups by asking their Principal Investigator to [add them by email or by scanning the Workgroup QR code](#).

When a user is added to a Workgroup by email, they are sent a [Notification](#) to confirm their addition to that Workgroup. Denying this request prevents the user from being added to the Workgroup.

Notifications

You Have Been Added to a Workgroup

A Principal Investigator has added you to the Workgroup, Development Workgroup, as a Standard Member. Please respond below.

Accept
Deny

2024-07-24 14:11:35.686611

5. Workbooks

Workbooks are collections of reactions intended to be from a single project. There can be multiple Workbooks within a Workgroup, and multiple users in a Workbook. Once a user is a member of a Workbook they can make, save, and reload reactions and add their own novel compounds. The Reactions in a Workbook can be viewed by selecting the corresponding Workbook from the dropdown on the [Workgroup page](#), or by selecting the Workbook from the Quick Access panel on the [home page](#).

5.1. Creating Workbooks

Workbooks can be created by Senior Researchers or Principal Investigators and can be done either from the Quick Access panel on the [home page](#) or from the [Manage Workbooks](#) page. When creating a new Workbook, you will be prompted to enter a Workbook name and 3 letter abbreviation for your Workbook – this abbreviation will form the basis for your Reaction Codes.

The screenshot shows the 'Create Workbook' form in the AI4Green application. The form is titled 'Create Workbook' and is located within the 'Development Workgroup'. It contains two input fields: 'Workbook Name' and 'Workbook Abbreviation'. Below the 'Workbook Abbreviation' field, there is a note: '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.' A 'Create Workbook' button is located at the bottom of the form. The top navigation bar includes links for Home, Demo, Solvents, Retrosynthesis, Workgroup, and Search, along with 'About AI4Green', 'Help', and 'User 1'.

Once created, your workbook will be visible in the Quick Access panel on the [home page](#) or visible from the Workbook dropdown on the [Workgroup Page](#).

5.2. Managing Workbooks

Senior Researchers and Principal Investigators can manage user membership in Workbooks. The Manage Workbook page is accessible from the [Workgroup page](#) if you have the correct membership level. The Workgroup is shown at the top of the page. New workbooks can be created by clicking the “Create Workbook” button.

Manage Workbooks

Workgroup Name: Development Workgroup

Select a workbook to begin:

Development-Workbook:1

Overview Requests

Name	Email	Action
Workbook Members		
Other Members in Workgroup		
User 1	user@mail.com	Add to Workbook
user 2	user2@mail.com	Add to Workbook

Create Workbook Export Workbook

AI₄Green Hazard Disclaimer | Privacy Notice | Twitter | GitHub Hazard data sourced from ECHA references on PubChem

Selecting a Workbook from the dropdown allows you to manage that Workbook. Users in the Workgroup can be added to the Workbook at any time. All Principal Investigators and Senior Researchers can manage all Workbooks within a Workgroup.

The data within the Workbook can be [exported](#) by clicking the “Export Workbook” button and ensuring you have selected the correct Workbook from the dropdown. Users can [request to join Workbooks](#), and their requests can be approved or denied under the request tab.

Home Demo Solvents Retrosynthesis Workgroup Search About AI4Green Help User 1

Manage Workbooks

Workgroup Name: Development Workgroup

Select a workbook to begin:
Development.Workbook-1

Overview Requests

Name	Email	Action
Workbook Members		
Other Members in Workgroup		
User 1	user@mail.com	+ Add to Workbook
User 2	user2@mail.com	+ Add to Workbook

Create Workbook Export Workbook

5.3. Joining Workbooks

Any Standard Member within a Workgroup can request to join a Workbook. For Standard Members, the “Join Workbook” button can be found on the [Workgroup page](#). Clicking this button allows you to see the active Workbooks in the Workgroup and send a request to join that Workbook. Different Workbooks can be selected from the dropdown.

Home Demo Solvents Retrosynthesis Workgroup Search About AI4Green Help Standard User

Request to Join a Workbook

Development.Workbook-1

Request to Join Workbook

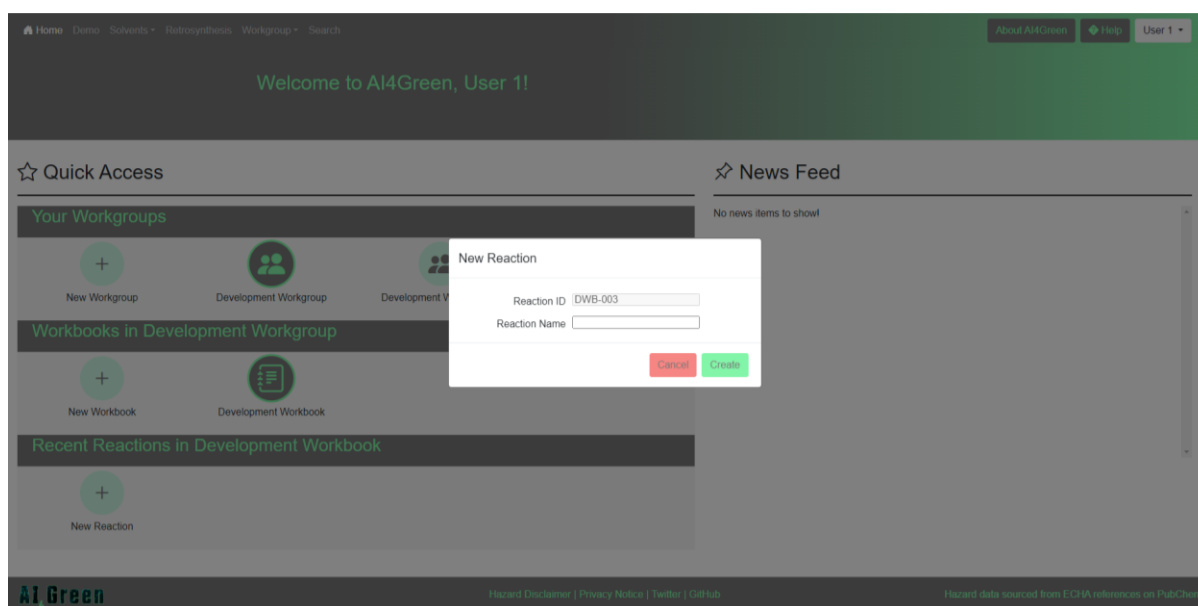
Principal Investigators and Senior Researchers have access to the [Manage Workbooks](#) page, so can be added to Workbooks from here.

Reactions

Reactions and reaction data are created and saved in their corresponding Workbooks. Members in a Workbook can view any Reaction in that Workbook, however only the creator of the Reaction can make changes to the Reaction.

5.4. Creating Reactions

New Reactions can be created either from the Quick Access panel on the [home page](#) or from the [Workgroup page](#). Each new reaction will be automatically assigned a reaction code using the Workbooks [three-letter abbreviation](#) and you will be asked to enter a name for the reaction. Clicking “Create” will take you to the [reaction constructor](#). The Reaction will then be visible in the Quick Access panel on the [home page](#) and the [Workgroup page](#).



5.5. The Reaction Constructor

The Reaction Constructor allows you to include all the necessary reaction data needed to carry out synthetic organic chemistry. This section will discuss in detail each of the sections of the reaction constructor. All changes made to Reactions are saved automatically. For a tutorial on how to use the reaction sketcher, please see the [tutorial page](#).

5.5.1. The Reaction Sketcher

AI4Green has two built in reaction sketchers for you to choose from. Both sketchers, either Marvin JS or Ketcher, allow you to draw out chemical structures and reactions as you would in a paper notebook. You can seamlessly switch between the two using the radio button at the top of the sketcher. Clicking the “Submit” button generates the [Reaction Table](#) that includes the information about your chemicals. The “Retrosynthesis” button connects you to out [AI powered retrosynthesis tool](#). See the corresponding sections to find out more.

At present, it is not possible to add reagents above the arrow. These must be entered separately in the [Reaction Table](#).

For more detailed guidance, please refer to the [MarvinJS](#) and [Ketcher](#) user manuals.

The screenshot displays the AI4Green Reaction Sketcher interface. At the top, there is a navigation bar with links for Home, Data, Subsets, Retrosynthesis, Workgroup, and Search. A user profile section on the right shows 'About AI4Green', 'Help', and 'User 1'. The main area is titled 'Example Reaction' with ID 'DWB-004'. It includes a prompt: 'Need some help getting started? Enter Tutorial Mode'. Below this, instructions state: '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.' The 'Selected Reaction Sketcher' is set to 'MarvinJS' (selected) and 'Ketcher'. The central workspace shows a chemical reaction: 4-aminophenol reacts with acetic anhydride to form N-(4-hydroxyphenyl)acetamide. A toolbar on the left contains drawing tools, and a vertical toolbar on the right contains element selection tools (H, C, N, O, S, P, Cl, Br, I, F, X). A hint at the bottom reads: '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'. At the bottom of the interface, there are buttons for 'Example', 'Submit', and 'Retrosynthesis', and a footer with 'AI Green', 'Hazard Disclaimer | Privacy Notice | Twitter | GitHub', and 'Hazard data sourced from ECHA references on PubChem'.

5.5.2. The Reaction Table

Once the reaction scheme has been submitted, the Reaction Table is generated. This is automatically populated with existing chemical data taken from [PubChem](#) or you Workbook’s [compound database](#). If any of your chemical structures are not recognised, you will be prompted to [add your compound to the compound database](#).

A description box is provided to include the details of the reaction procedure and any other important information that is not included in the Reaction Table. The Reaction Class is also automatically identified, and this is important information for the [Solvent Surfer](#) selection tool. While we make every effort to ensure the reaction class is correctly identified, it can make mistakes. Please confirm that this is correct before proceeding.

The Reaction Table can be edited. The boxes with the red outline indicate which fields are required to be inputted by the user. The mass of the limiting reactant and equivalents of all other reactants are needed to automatically calculate the values. The equivalent of the limiting reactant is always 1, and the others should be chosen relative to this. Physical forms for each component can be chosen via a dropdown menu. These contribute to the overall risk rating of each chemical and the overall Reaction, which is shown in the [Summary Table](#).

Example Reaction

Please describe your reaction

Please fill in the highlighted boxes to proceed

Reaction Class: Amide bond formation

Nr	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	-	-	1	-	-	-	-select-	H302-H315-H318-H319-H335-H372
2	Ethylamine	<input type="radio"/>	45.08	-	-	-	-	-	-	-select-	H220-H280-H302-H311-H314-H318-

Catalysts/reagents
Add new reagent to database

Solvents
Add new solvent to database

Product **Desired Product?**

3	N-Ethylbenzamide	<input checked="" type="radio"/>	149.19	-	-	-	-	-	-	-select-	H302
---	------------------	----------------------------------	--------	---	---	---	---	---	---	----------	------

Summary

AI₄Green Hazard Disclaimer | Privacy Notice | Twitter | GitHub Hazard data sourced from ECHA references on PubChem

If there is more than one product, you may choose which is the desired product. This is important for the automatic calculation of the percentage yield.

[Reagents](#) and [solvents](#) must be added separately using the “Add Reagent” and “Add Solvent” buttons.

The amounts are automatically calculated from your input. Once all relevant fields have been filled in (and these fields will be highlighted red until they have been filled), the reaction table is complete, and a summary table can be produced by clicking “Summary”. Further information about the input fields is given below.

Reagents

Reagents can be added by clicking on the “Add Reagent” button. Entering their name or CAS number will search the database for the desired compound and automatically update the hazard information. If no reagent is returned, it is not in the PubChem database and needs to be added via the sketcher or using the “Add new reagent to database” button. You may need to manually enter the density of any liquids.

The number of equivalents and physical form are also required for reagents.

Catalysts/reagents		
Add new reagent to database		
3	Name or CAS Number	select...

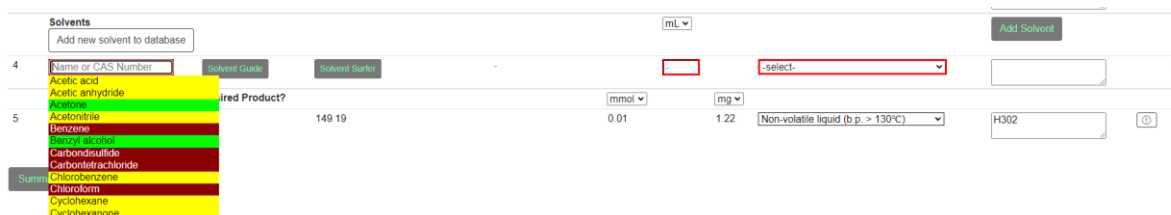
Solvents

Clicking the “Add Solvent” button opens a searchable interactive dropdown. Novel Solvents can be easily [added to the database](#) in a similar way to Novel Compounds.

Here each solvent is colour coded based upon green metrics from CHEM21. Green colour means recommended solvents, yellow means problematic, red means hazardous, and maroon means highly hazardous (these will differ if the user has changed them under the accessibility options). Solvents can also be searched for by entering their CAS number.

The volume and physical form are required here.

The “Solvent Guide” and “Solvent Surfer” buttons easily connect you to AI4Green’s solvent selection tools, the [Solvent Guide](#) and [Solvent Surfer](#). Please see these sections to find out more.



5.5.3. Compound Database

If you have drawn a molecule that is not included in the PubChem database, you will be prompted to enter it as a novel compound. Doing this will ensure that you can reuse this compounds information in future reactions. Each Workbook has an associated novel compound database, so no users outside your Workbook will be able to see your novel compounds.

To add a novel compound, you will be prompted to provide as much information as possible regarding this compound. Once done, click ‘Input’.

Reactant 1 not in database.

Name: MW: Hazard Codes: CAS: Density (g/mL):

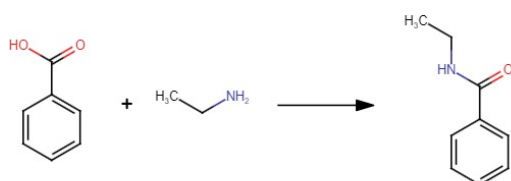
Conc. (M):

*IUPAC names are auto-generated by [Chemical Identity Resolver](#) and [STOUT](#)

The SMILES string from the Reaction Sketcher will be used to try and generate the IUPAC name of the molecule, but this is not always possible. In this case, the user must give the molecule a name. The molecular weight will be automatically calculated and filled in. Hazard codes for novel compounds should be entered using a dash as a delimiter, e.g., ‘H301-H331-H302’.

5.5.4. Summary Table

Once the Reaction Table is complete you can generate a summary of the reaction. This includes all chemicals and their amounts, as well as providing a breakdown of the chemical hazards. The Summary Table requires the user to input the unreacted mass of starting material and the mass of the product once the reaction is finished to calculate the percentage yield.



No	Reactants/catalysts/reagents	Mol.Wt	Density (g/mL)	Conc. (M)	Equiv.	Amount (mmol)	Volume (μL)	Mass (mg)
1	Benzoic acid	122.12			1	0.82	0.00	100
2	Ethylamine	45.08	0.7		3	2.46	157	111
3	Diisopropylethylamine	129.24	0.742		1.4	1.15	200	148
4	O-(7-Azabenzotriazol-1-yl)-N,N,N',N'-tetramethyluronium hexafluorophosphate	380.23			1.2	0.98	0.00	374
							Volume (mL)	
5	Ethyl acetate						2	
Product		Mol.Wt	Theoretical Yield (mg)	Unreacted	Product Mass (mg)	% Yield		
6	N-Ethylbenzamide	149.19	122	<input type="text" value="-"/>	<input type="text" value="-"/>			

	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, H318 Causes serious eye damage, H331 Toxic if inhaled, H335 May cause respiratory irritation	VH	M	VH
4	H228 Flammable solid, H315 Causes skin irritation, H317 May cause an allergic skin	VH	L	H

There is also some additional safety and sustainability information to enter to calculate the green metrics for your reaction. This is where you can record the temperature, the reactor type (batch/flow), isolation method, stoichiometry and catalyst recovery steps. These all give a sustainability score which is colour coded to provide an easy visualisation.

Sustainability (CHEM21)							
Solvents	Safety	Temp °C	Elements	Batch/flow	Isolation	Catalyst	Recovery
Ethyl acetate	H1	120	+500 years	Batch	Column	No catalyst	-select-
	Atom Efficiency	Mass Efficiency	Yield	Conversion	Selectivity		
	22.0	10.7	74	90	82		
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"/> Ozone				
<input type="checkbox"/> Free Radicals	<input type="checkbox"/> Liquid Ammonia	<input type="checkbox"/> Peroxides	<input type="checkbox"/> Sealed Tube				
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							
<small>(Hazardous by Products, Exothermic reactions, The need to inform others of risks, Lab and hood number.)</small>							
<input type="text"/>							
Hazard categorisation given GLP and other controls specified							
Hazard <i>Potential to cause harm</i>	<input type="radio"/> 1. Slight <input checked="" type="radio"/> 2. Serious <input type="radio"/> 3. Major	Risk Category (A-D) <input type="radio"/> A (10-27)	Risk Score HxRxC				
Risk <i>Likelihood of exposure</i>	<input checked="" type="radio"/> 1. Low likelihood <input type="radio"/> 2. Possible <input type="radio"/> 3. Frequent Occur	<input type="radio"/> B (6-9)	<input type="text" value="2"/>				
Consequences <i>Who will be affected</i>	<input checked="" type="radio"/> 1. Individual <input type="radio"/> 2. Local Labs <input type="radio"/> 3. Building wide	<input type="radio"/> C (3-5) <input checked="" type="radio"/> D (1-2)					
Signed: _____							

Finally, a hazard assessment is required to ensure you have considered the physical and chemical hazards of your procedure. This must be [printed](#) and signed off by the researcher and the supervisor before any reactions are undertaken in the laboratory.

Printing the Summary Table

The print summary button will allow you to print the summary table. This contains the reaction scheme, Reaction Table, hazard matrix, sustainability metrics, additional hazard data, and space for the chemist's and their supervisor's signature.

This printout can be taken into the lab and placed near the reaction to act as a reference for the COSHH + H&S data for the reaction. If you are using this as a risk assessment in the laboratory, it MUST be signed off by both you and your supervisor.

test
Owner: PL_Dummy

Reagents/catalysts/reagents	Mol.Wt	Density (g/mL)	Conc. (M)	Eqivs.	Amount (mmol)	Volume (mL)	Mass (mg)
1 Benzoic Acid	122.12			1	0.02	0.00	2
2 Ethylamine	45.08			2	0.03	0.00	1.48

Solvents	Volume (mL)
3 Acetic acid	2

Product	Mol.Wt	Theoretical Yield (mg)	Unreacted	Product Mass (mg)	% Yield
4 N-Ethylbenzamide	145.19	2.44	0.1	0.2	82

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 H228 Extremely flammable gas, H318 Causes serious eye irritation, H330 May cause respiratory irritation	H	M	H
3 H228 Flammable liquid and vapor, H260 May be corrosive to metals, H314 Causes severe skin burns and eye damage	H	M	H
4 H302 Harmful if swallowed	M	M	M

Sustainability (CHEM21)	Safety	Temp °C	Elements	Batch/flow	Isolation	Catalyst	Recovery
Acetic acid	H	25	C, O	Batch	None	None	Not recovered catalyst
Atom Efficiency	93.2						
Yield	82						
Conversion	93						
Selectivity	93						

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.
(Hazardous by Products, Exothermic reactions. The need to inform others of risks. Lab and hood number.)

5.5.5. Polymer Mode

NEW TO AI4GREEN

Polymer mode allows you to draw repeating units in the sketcher and pass them to the reaction table. Polymer mode can be activated by checking the “Polymer Mode” checkbox shown at the top of the sketcher, indicated below by the red box.

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polymer example
DW1-043
Need some help getting started?
[Enter Retrosyn 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.

Polymer Mode?

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

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There are a few differences between polymer mode and the standard reaction constructor. These include drawing structures, the reaction table and the summary table.

The Reaction Sketcher

Please note that the MarvinJS sketcher cannot be used with polymer mode. To draw a polymer in the sketcher, select the [S] tool from the ketcher toolbar and highlight repeating of your structure.

This tool will bring up the “S-Group properties” dialogue box, and polymers can be marked by selected “SRU Polymer” from the Type dropdown. SRU stands for Structural Repeating Unit. Selecting SRU polymer encloses the highlighted atoms within square brackets, which can be given a label by filling in the “polymer label” input field. There are three types of repeat patterns: head-to-tail (default), head-to-head, and either/unknown. These can be selected from the “Repeat pattern” dropdown and each one will cause a different visualisation in the sketcher. We recommend selecting head-to-tail, but all types are handled in the same way.

When clicking submit, you will have to input the name of your polymer.

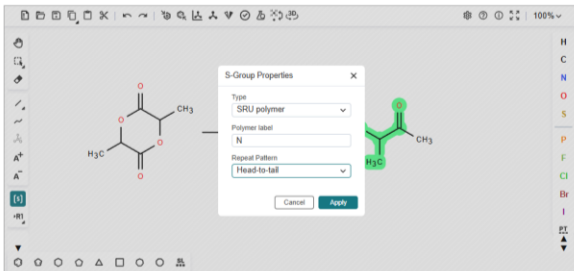
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Need some help getting started?
[Enter Tutorial Mode](#)

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.

Polymer Mode?

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](#)

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The Reaction Table

The reaction table is mostly the same as the standard reaction constructor, though the molecular weight is provided for the repeating unit only. A new drop down is also generated, in which you can specify the type of polymerisation.

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[Example](#) [Submit](#) [Retrosynthesis](#)

polymer example

Please describe your reaction

Type of polymerisation:

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	Lactide, DL-	<input type="checkbox"/>	144.12	-	-	<input type="text" value="1"/>	0.69	0.00	100	<input type="text" value="Dense solid"/>	<input type="text" value="H319"/>
<p>Catalysts/reagents <input type="text" value="Add new reagent to database"/> Add Reagent</p> <p>Solvents <input type="text" value="Add new solvent to database"/> <input type="text" value="mL"/> Add Solvent</p>											
2	Poly(lactic acid)	<input type="checkbox"/>	144.13 Repeating unit	-	-	-	<input type="text" value="0.69"/>	<input type="text" value="100"/>	<input type="text" value="100"/>	<input type="text" value="Dense solid"/>	<input type="text" value="Unknown"/>

[Summary](#)

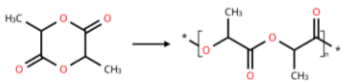
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The Summary Table

The summary table remains the same as the standard reaction summary, but the input fields for experimental data are different. The unreacted mass and percentage yield can still be recorded, but extra fields for the number-averaged and weight-averaged molecular weights,

dispersity, glass transition temperature, melting temperature and crystallisation temperature are provided.

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No	Reactants/catalysts/reagents	Mol.Wt	Density (g/mL)	Conc. (M)	Equiv.	Amount (mmol)	Volume (mL)	Mass (mg)
1	Lactide, DL-	144.12			1	0.69	0.00	100

Solvents		Volume (mL)

Product	Mol.Wt	Theoretical Yield (mg)	Unreacted	Product Mass (mg)	% Yield
2 Poly(lactic acid)	144.13	100			

Polymer Characterisation:

Mass	M _n	M _w	Dispersity	Measurement Method	Calibration standard
				select	

Thermal Properties	T _g	T _m	T _c	Measurement Method	Calibration standard
				select	

Hazards	Hazard Rating	Exposure Potential	Risk Rating
1 H319 Causes serious eye irritation	M	L	L
2 Unknown Treat as toxic	M	L	L
		Risk Rating:	M

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5.5.6. Uploading Experimental Data

After the Reaction has been carried out in the lab, you can choose to upload any experimental or analytical data to AI4Green in addition to the reaction yield.

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(Hazardous by Products, 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	<input type="radio"/> 1. Slight <input type="radio"/> 2. Serious <input type="radio"/> 3. Major	Risk Category (A-D) <input checked="" type="radio"/> A (10-27)	Risk Score HxRxC
Risk Likelihood of exposure	<input type="radio"/> 1. Low likelihood <input type="radio"/> 2. Possible <input type="radio"/> 3. Frequent Occur	<input checked="" type="radio"/> B (6-9)	
Consequences Who will be affected	<input type="radio"/> 1. Individual <input type="radio"/> 2. Local Labs <input type="radio"/> 3. Building wide	<input checked="" type="radio"/> C (3-5) <input type="radio"/> D (1-2)	

Signed:

Researcher: Supervisor:

Upload Experimental Data

Choose files No file chosen Upload

Lock Reaction

Print Summary

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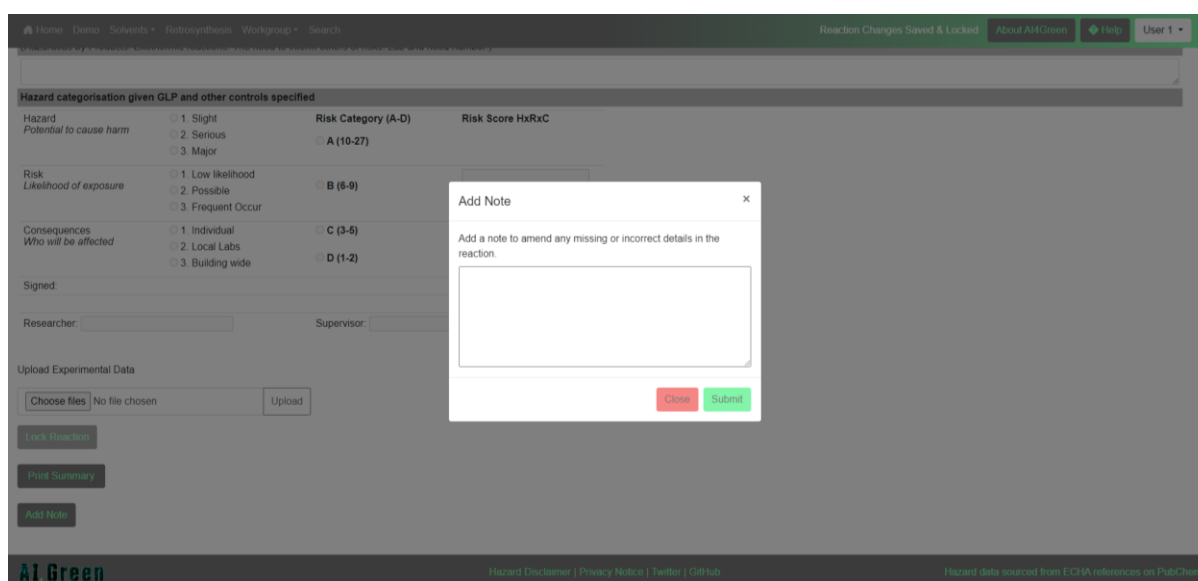
Only files with the following extensions can be added at this time:

.arw, cif, .cdf, .cdx, .csv, .D, .dat, .DTA, .dx, .fid, .gz, .jpg, .jdx, .jcamp, .mnova, .pdf, .pkl, .png, .pdb, .psession, .qgd, .raw, .res, .topspin, .txt, .vrml, .xlsx, xls, .xyz, .zip

If you require any additional file extensions, please let us know by emailing the AI4Gree team at admin@ai4green.app

5.6. Completing a Reaction

Once all the fields of a reaction have been filled in, the Reaction should be locked to prevent any further changes. Note that a reaction cannot be unlocked, but notes can be added if any other information is required later. The time and date of the note is displayed alongside the content at the bottom of the Reaction Constructor.



5.7. Saved Reactions

All changes made to a Reaction are saved automatically. Saved Reactions can be viewed and reloaded from either the Quick Access panel in the [home page](#) or in the [Workgroup page](#).

On the Workgroup page, users can view all Reactions in the workbook and order them either alphabetically or by date created. Each Reaction is summarised with its reaction scheme, the date of creation, whether the Reaction is [locked](#) and whether the Reaction contains any [notes](#) (amendments).

Clicking the “Reload” button will allow you to load that Reaction in the [Reaction Constructor](#). The “Delete” button will archive your Reaction. This means that it will no longer be visible in your Workbook but will still be recoverable in case of accidental deletion. The “Clone” button allows you to create a new Reaction using all the information from the Reaction you clone. The chemicals and their amounts can still be changed in the [Reaction Table](#).

5.8. Tutorial


A step-by-step guide for the [Reaction Constructor](#) is available on the [Help](#) page which is accessible from the [Navigation bar](#).

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AI4Green Documentation & Help

Video Tutorials

We have several video tutorials to explain Workgroups & Workbooks, the Reaction Constructor, and our Solvent Guide. Click the icon in the top right of the player to view all videos in this playlist.



Watch on YouTube

User Guides

- Quickstart Guide
- User Guide
- Marvin JS Help Page
- Reaction Builder Tutorial **SP**

Click here to view the [privacy notice](#).
Click here to view the [hazard disclaimer](#).

GitHub Repository

For further help, queries or suggestions please feel free to contact us: ai4green@nottingham.ac.uk.

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Clicking the “Reaction Builder Tutorial” button initiates the tutorial, which guides you through each of the elements.

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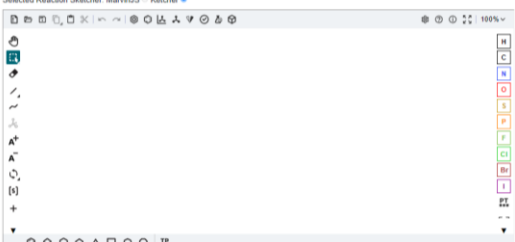
Tutorial Reaction

TUT-001

Need some help getting started?
[Enter Tutorial Mode SP](#)

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](#)

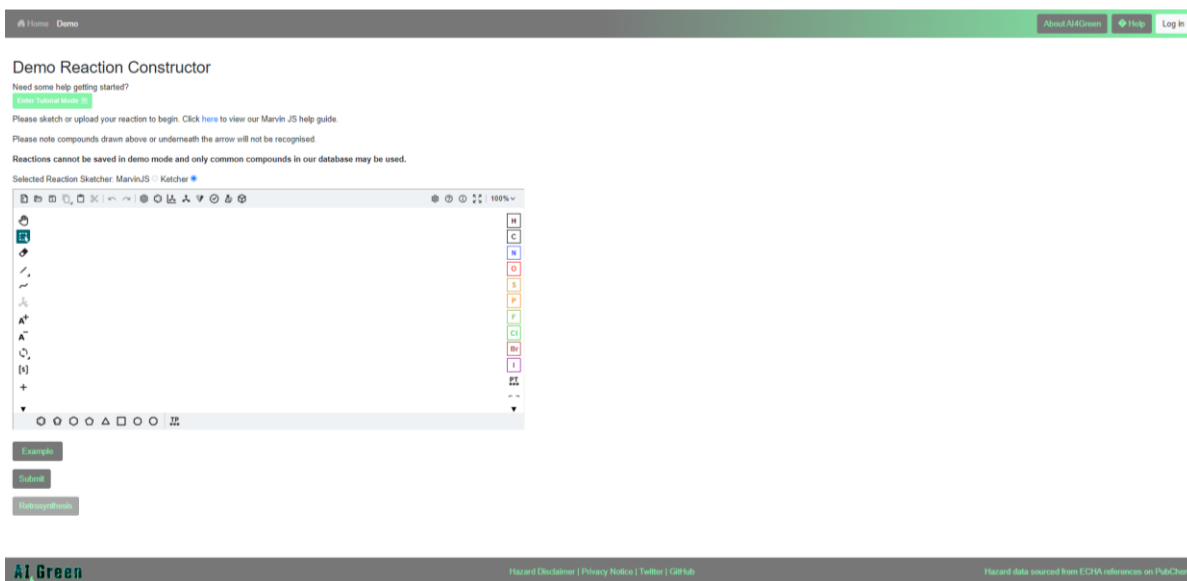
AI Green Hazard Disclaimer | Privacy Notice | Twitter | GitHub Hazard data sourced from ECHA references on PubChem

Welcome to the reaction sketcher tutorial
This tutorial leads you through the key steps in building a reaction

[Back](#) [Next](#)

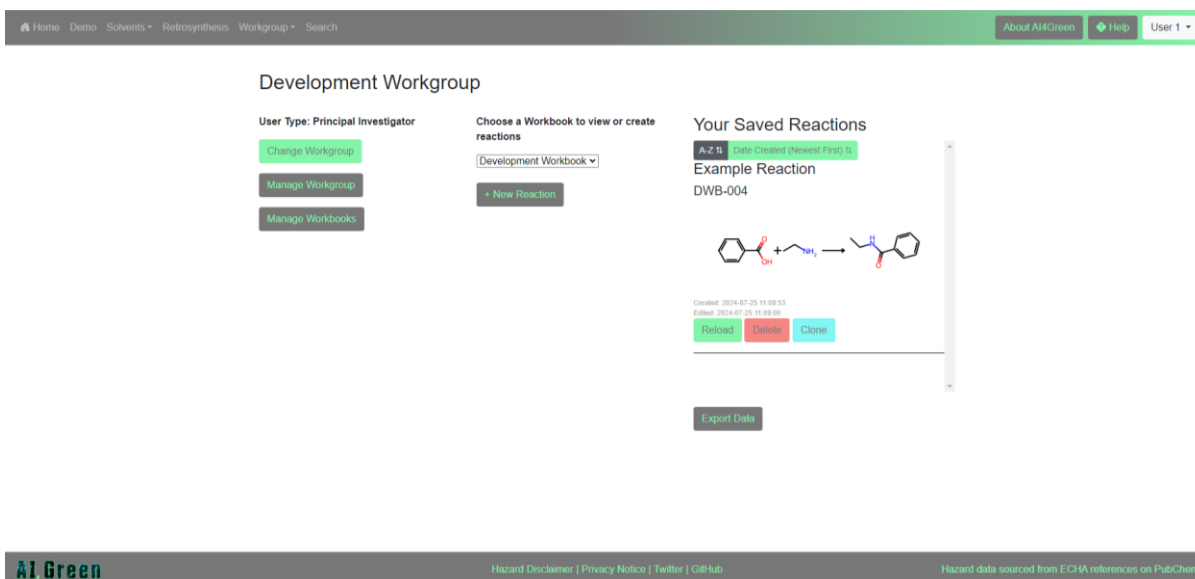
5.9. Demo

The Demo link in the [Navigation bar](#) allows you to try out the Reaction Constructor without needing an AI4Green account. Note that you will not be able to access the Retrosynthesis feature without an account.



5.10. Exporting Data

Reaction data in a [Workbook](#) can be exported from the [Workgroup page](#), below the list of [saved reactions](#) on the right side by clicking the “Export Data” button.



This takes you to the Export Data page, which allows you to export your data in different human and machine-readable formats. All Workbook members have permission to export data from their Workbooks, and Principal Investigators can export from any Workbook in their

Workgroup. Note that reactions updated before version 1.5 may not have all information exported.

The screenshot shows the 'Data to Export' interface in AI4Green. It includes a navigation bar with 'Home', 'Demo', 'Solvents', 'Retrosynthesis', 'Workgroup', and 'Search'. On the right, there are links for 'About AI4Green', 'Help', and 'User 1'. The main content area is divided into two columns. The left column, titled 'Data to Export', contains dropdown menus for 'Workgroup' (set to 'Development Workgroup') and 'Workbook' (set to 'Development Workbook'). Below these is a 'Select Reactions' button and a note: 'Only reactions with a recorded yield are available for export.' The right column, titled 'Select Export Format', lists 'Machine-Readable Formats' (JSON, RDF, ELN) and 'Human- and Machine-Readable Formats' (CSV, SURF [1]). A 'References' section at the bottom provides a link to a paper: '[1] Simple User-Friendly Reaction Format, Chemrxiv, 2023, DOI: 10.26434/chemrxiv-2023-nfq7h'. The footer contains the AI4Green logo, a 'Hazard Disclaimer | Privacy Notice | Twitter | GitHub' link, and a note: 'Hazard data sourced from ECHA references on PubChem'.

You can choose which Reactions in a Workbook you want to export by clicking the “Select Reactions” button. Simply clicking on the reaction code toggles it between Included or Excluded. Only [Reactions](#) with a percentage yield will be eligible for export.

This screenshot shows the same 'Data to Export' interface as above, but with a 'Select Reactions' modal window open in the center. The modal has a title bar with a close button (X) and two columns: 'Excluded' and 'Included'. Under 'Excluded', there is a text input field containing 'DWB-005'. Under 'Included', there are two text input fields containing 'DWB-003' and 'DWB-006'. The background interface is dimmed. The footer is identical to the previous screenshot.

Each attempt to export data from a Workbook must be approved by a Principal Investigator. Each Principal Investigator in the Workgroup will receive a notification with the details of the

export request: the user, time and date, Workbook and export format. The Principal Investigator must then approve this request before the export is ready. Once approved, the data export will expire after 7 days.

5.10.1. Export File formats

There are several different formats to export your data into. A brief explanation of each is given here.

JSON

JSON stands for JavaScript Object Notation and is often used for transferring data between web pages and their servers. The Reaction data is stored as a series of dictionaries.

RDF

RDF stands for Reaction Data File and is a standard format for storing reactions in chemistry. This is an extension of the [RXN](#) file that includes metadata.

ELN

ELN files were introduced by the ELN Consortium and provides interoperability between different ELNs. The ELN files allows you to extract your data from AI4Green and load it into any other ELN that is a member of the ELN consortium. This file includes both RXN and JSON.

CSV

CSV stands for Comma Separated Values and is a type of file associated with spreadsheet format. Each row of the spreadsheet contains one Reaction and its metadata. These files can be opened in Excel.

SURF

SURF stands for Simple User-Friendly Reaction Format and standardises reaction data using structured tables. This format compliments the storage of reaction data as seen in the Open Reaction Database.

RXN

This file stores Reactions as reaction blocks, which are lists of a reaction's atoms and their connectivities.

6. Solvent Selection

The AI4Green solvent selection tools are accessible from the Solvents dropdown in the [Navigation bar](#). There are two such tools, the [Solvent Guide](#) and the [Solvent Surfer](#).

6.1. Solvent Guide

The Solvent Guide is a set of solvent flashcards that provide a visual summary of solvent information for quick and easy comparison of solvents. Solvents are organised by functional group and selecting a solvent displays its flashcard. Up to two flashcards can be viewed at a time making it easy to compare. The hazard colours can be changed via the [accessibility](#) page. A breakdown of all the information provided by the flash cards is available by clicking the “About the Solvent Guide” button. A [standalone version of the Solvent Guide](#) is available.

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Solvent Guide

About the Solvent Guide Solvent Surfer

Choose up to two solvents from the classes below to compare them

- Acids
- Alcohols
- Amines
- Aprotic polar
- Esters
- Ethers
- Halogenated
- Hydrocarbons
- Ketones
 - Acetone
 - Cyclohexanone
 - Methyl ethyl ketone
 - Methyl isobutyl ketone
- Miscellaneous
- Water

Acetone
Recommended

CAS: 67-64-1
Family: Ketones
Boiling Point / °C: 56
Flash Point / °C: -18

Safety: 3
Health: 5
Environment: 5
Worst HDxx: H319G
Worst HDxx: G

Issues: na
Possible Substitution(s): No Substitutions Found

Cyclohexane
Problematic

CAS: 110-82-7
Family: Hydrocarbons
Boiling Point / °C: 81
Flash Point / °C: -17

Safety: 3
Health: 5
Environment: 5
Worst HDxx: H226G
Worst HDxx: H410B

Issues: na
Possible Substitution(s): No Substitutions Found

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The solvent guide can be accessed from the [Navigation bar](#) or by clicking the “Solvent Guide” button when [adding solvents to a reaction](#). The latter option will load the selected solvent in the Solvent Guide for easy comparison.

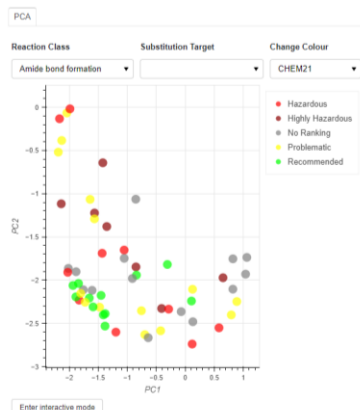
6.2. Solvent Surfer

The Solvent Surfer is a solvent selection tool that applies Principal Component Analysis (PCA) to a set of 16 physicochemical solvent descriptors to identify solvents with similar properties. The descriptor set can be tailored depending on the reaction class, including only the most important descriptors for that reaction.

Upon loading the Solvent Surfer page, you are prompted to select a reaction class which generates the corresponding PCA plot.

Information about the reaction class and an explanation of which descriptors were used and why is provided under the Reaction Class tab. Each data point on the PCA graph is a solvent and these are colour-coded according to their CHEM21 sustainability scores. The colour-coding can be changed via the [accessibility](#) page.

Solvent Surfer



Suggested Solvents Reaction Class Saved Graphs About

Amide Bond Formation

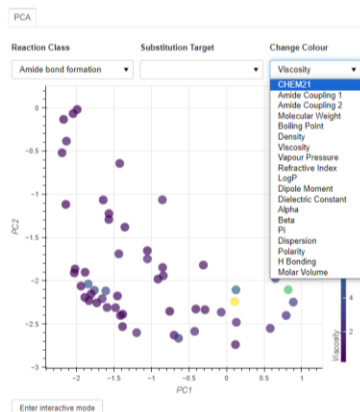
Amide bond formation is a condensation reaction between carboxylic acids and amines. Typically, a coupling agent and base are required.

$$R^1-COOH + H_2N-R^2 \xrightarrow[\text{Base}]{\text{Coupling Reagent}} R^1-CO-NH-R^2 + H_2O$$

Common coupling reagents

The colours of the data points can also be changed to reflect any of the initial PCA descriptors by selecting a value from the “Change Colour” dropdown. Some experimental data is also included as a colour, and the details of these are provided under the Reaction class tab.

Solvent Surfer



Suggested Solvents Reaction Class Saved Graphs About

Hydrogen Bonding δ_s

Experimental Data

Amide Coupling 1

A study by [Macmillan et al.](#)¹ monitored the effect of solvent on % conversion of the reaction below after 4 hours. This data can be viewed by selecting **Amide Coupling 1** in the Change Colour dropdown.

$$Ph-CH_2-COOH + H_2N-CH_2-C_6H_4-OMe \xrightarrow[\text{Solvent, rT}]{\text{HATU (1.2 eq.)}, \text{Pr}_2\text{NEt (2 eq.)}}$$

Amide Coupling 2

A different amide bond formation reaction was studied by [Kunshima et al.](#)² The % yield was measured for a range of solvents. This data can be viewed by selecting **Amide Coupling 2** in the Change Colour dropdown.

$$CH_3OH + CH_2=CH-CH_2-NH-C_6H_4-OMe \xrightarrow[\text{NCHM (1.0 eq.)}]{\text{CDMT (1.1 eq.)}}$$

The cost, melting point and boiling point of each solvent can be viewed by hovering over the datapoints and clicking a datapoint or selecting a solvent from the “Substitution Target”

dropdown generates a table of solvents that are closest to the chosen solvent under the “Suggested Solvents” tab.

More information about the Solvent Surfer is available under the “About” tab.

6.2.1. Interactive Mode

Interactive mode allows users to directly interact with the PCA visualisation by clicking and dragging data points into new positions. This uses [interactive knowledge-based kernel PCA](#) to adjust the PCA embedding according to the placement of the dragged points, allowing users to explore many different PCA embeddings. Interactive mode can be used to group solvents that give similar experimental results for a given use case (solubility measurements, percentage yield, etc) providing a more specific and relevant embedding.

Interactive mode can be activated by clicking the “Enter Interactive Mode” button. Once activated, you are then able to move the data points by clicking and dragging them into new positions. When points are dropped, the embedding is automatically updated to reflect this. The moved points are circled by red to indicate these have been moved.

Interactive Surfers can be saved by clicking the “Save” button, where you will be prompted to enter a name for your updated graph. Saved Surfers can be viewed under the “Saved Graphs” tab. These can easily be reloaded or deleted. Note that deleted graphs are archived, so while they are no longer seen under the “Saved Graphs” tab, they are recoverable.

Updated graphs can be reset using the “Reset” button, which reverts the PCA graph back to its original state. This cannot be undone, so please ensure any saved changes are made before clicking this button.

To interrogate the updated plot, you must first exit interactive mode. Then, you can generate the Suggested Solvent table as before, by clicking on any data point or selecting a target from the “Substitution Target” dropdown.

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Solvent Surfer

PCA

Reaction Class: Amide bond formation Substitution Target: Methanol Change Colour: CHEM21

Enter interactive mode

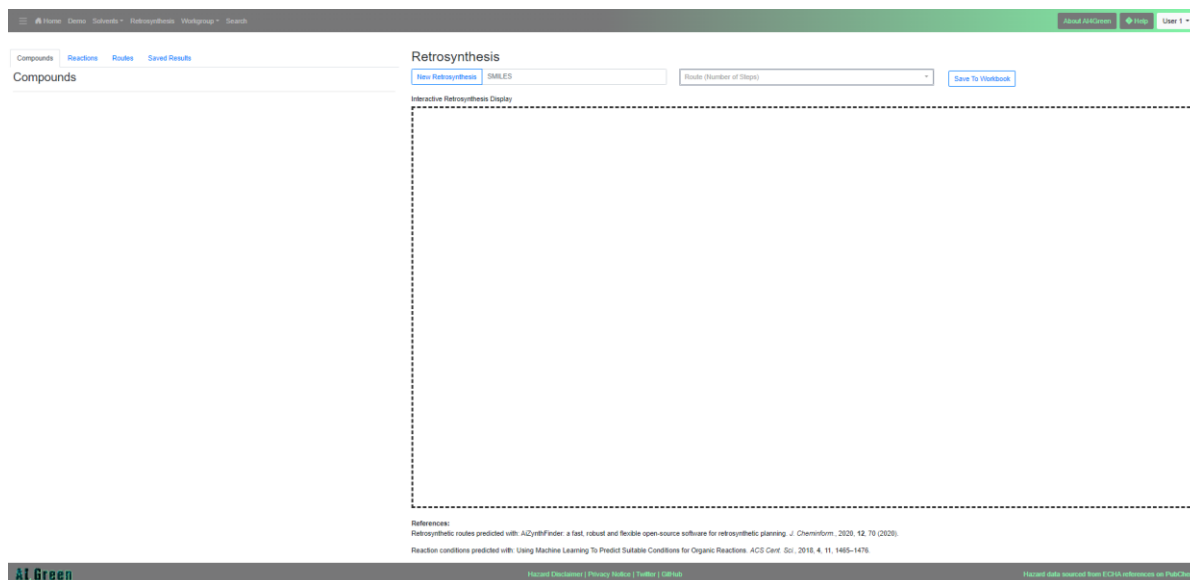
Suggested Solvents Reaction Class Saved Graphs About

#	Solvent	Distance	CHEM21 Ranking
0	Methanol		Recommended
1	Hexafluoroisopropanol	0.13	No Ranking
2	Acetonitrile	0.14	Problematic
3	Trifluoroethanol	0.14	No Ranking
4	Ethanol	0.28	Recommended
5	Acetone	0.30	Recommended
6	Nitromethane	0.31	Highly Hazardous
7	Acetic acid	0.38	Problematic
8	Isopropyl alcohol	0.39	Recommended
9	i-Butanol	0.49	No Ranking
10	Water	0.50	Recommended
11	t-Butanol	0.51	Recommended
12	Dichloromethane	0.51	Hazardous
13	Methyl ethyl ketone	0.52	Recommended
14	i-Amyl alcohol	0.58	No Ranking
15	2-Methoxyethanol	0.61	Hazardous
16	Acetic anhydride	0.63	Problematic
--	--	--	--

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7. Retrosynthesis

The Retrosynthesis tab can be accessed from the [Navigation bar](#) or when [building a Reaction](#). The latter option will preload either a single drawn molecule or product from the sketcher into the SMILES input field.



7.1. How it Works

To begin a retrosynthesis, enter the SMILES string of the target molecule into the input field and click submit. This will send the SMILES string to an instance of [AiZynthFinder](#), a software that uses machine learning to predict retrosynthetic routes. These retrosynthetic routes are converted to forward reactions. The conditions for these reactions are then predicted using [ASKCOS](#) which uses a machine learning algorithm to predict reaction conditions. This data is then used to make a sustainability assessment using the CHEM21 sustainability metrics. The sustainability metrics can be weighted by the user to update the weighted median sustainability of reactions and routes. This process usually takes up to 5 minutes.

If a route is found, the user will be able to see the retrosynthetic route displayed as a series of interactive nodes with the target molecule at the top of the tree and starting materials at the bottom.

A dropdown with a list of up to ten routes is colour-coded by their sustainability and number of steps in brackets. Different routes can be explored by clicking one of the options from the dropdown.

Retrosynthesis

Interactive Retrosynthesis Display

Route 1 (2) [Yellow]

Route 2 (2) [Yellow]

Route 3 (2) [Yellow]

Route 4 (2) [Yellow]

Route 5 (2) [Yellow]

Route 6 (2) [Yellow]

Save To Workbook

References:
 Retrosynthetic routes predicted with: AI2YrBFinder, a fast, robust and flexible open-source software for retrosynthetic planning. *J. Cheminform.* 2020, 12, 70 (2020).
 Reaction conditions predicted with: Using Machine Learning To Predict Suitable Conditions for Organic Reactions. *ACS Cent. Sci.* 2018, 4, 11, 1465-1476.

7.2. Analysis

A series of tabs on the left sidebar provide additional analysis of the predicted routes. Changing routes or clicking a molecule will dynamically alter the contents of these tabs.

The **compound** tab draws from the AI4Green database to show CAS number, name, hazards, and molecular weight.

Retrosynthesis

Interactive Retrosynthesis Display

Compound	
Name	Picolinic acid
Molecular Weight	123.11
CAS	95-95-8
Hazard Codes	H302-H315-H318-H319-H332-H335

References:
 Retrosynthetic routes predicted with AI₂ynthFinder: a fast, robust and flexible open-source software for retrosynthetic planning. *J. Cheminform.* 2020, 12, 70 (2020).
 Reaction conditions predicted with: Using Machine Learning To Predict Suitable Conditions for Organic Reactions. *ACS Cent. Sci.* 2016, 4, 11, 1465-1476.

The **reaction** tab displays the predicted conditions to make the clicked molecule including temperature, reagents, solvent, catalyst, and hazards. Additionally, the sustainability metrics for the reaction are colour-coded, including temperature, stoichiometry, atom economy, and hazards. There is also a dropdown where alternative conditions can be evaluated.

Reactions

Condition Set 1

Conditions & Sustainability	
Temperature (°C)	122
Solvent	No solvent
Reagents	CC(C)O[D]LH
Stoichiometry/Catalyst	No catalyst
Element Sustainability	65-999 years
Atom Economy	72.8%
Safety	No Hazard/Toxic Issues

Export to Sketcher

References:
 Retrosynthetic routes predicted with AI₂ynthFinder: a fast, robust and flexible open-source software for retrosynthetic planning. *J. Cheminform.* 2020, 12, 70 (2020).
 Reaction conditions predicted with: Using Machine Learning To Predict Suitable Conditions for Organic Reactions. *ACS Cent. Sci.* 2016, 4, 11, 1465-1476.

Reactions can be exported to the sketcher from the reaction tab. This allows you to create a new Reaction in your workbook.

The screenshot shows the 'Retrosynthesis' tab in the AI4Green software. A 'New Reaction' dialog box is open, allowing the user to create a new reaction entry. The main interface displays a reaction scheme for the synthesis of a complex molecule. Below the reaction scheme, there is a table for 'Conditions & Sustainability' for 'Condition Set 1'.

Conditions & Sustainability	
Temperature (°C)	122
Solvent	EtOAc
Reagents	CCl ₄ /C(=O) [L=]
Stoichiometry/Catalyst	No catalyst
Element Sustainability	56-90 years
Atom Economy	72.9%
Safety	No Hazard Index Score

References:
 Retrosynthetic routes predicted with AI₂ynthFinder: a fast, robust and flexible open-source software for retrosynthetic planning. *J. Cheminform.* 2020, 12, 70 (2020).
 Reaction conditions predicted with: Using Machine Learning To Predict Suitable Conditions for Organic Reactions. *ACS Cent. Sci.* 2018, 4, 11, 1465-1476.

The **route** tab displays an overview of the sustainability of each reaction step for each metric. This is also where the sliders are to adjust the weightings of the metrics which updates the weighted median used to colour reactions and routes.

When calculating the sustainability metrics, we assume 1.0 equivalent of reagents and 0.05 equivalents of catalyst are used.

The screenshot shows the 'Routes' tab in the AI4Green software. It displays a table for 'Step Analysis' comparing two routes (1 and 2) across various sustainability metrics. The 'Routes' section also includes a 'New Retrosynthesis' dialog box and a reaction scheme.

Step Analysis	1	2
Solvent	Green	Green
Temperature	Green	Green
Stoichiometry/Catalyst	Yellow	Yellow
Element Sustainability	Red	Green
Atom Economy	Green	Green
Safety	Green	Green
Weighted Median	Green	Yellow

Adjust Sustainability Metric Weightings:
 Solvent: Default
 Temperature: Default
 Stoichiometry/Catalyst: Default
 Elements: Default
 Atom Economy: Default
 Safety: Default

References:
 Retrosynthetic routes predicted with AI₂ynthFinder: a fast, robust and flexible open-source software for retrosynthetic planning. *J. Cheminform.* 2020, 12, 70 (2020).
 Reaction conditions predicted with: Using Machine Learning To Predict Suitable Conditions for Organic Reactions. *ACS Cent. Sci.* 2018, 4, 11, 1465-1476.

Additional Features

Results can be saved to a workbook by clicking the “Save To Workbook” button. All members of that workbook members will be able to see and reload these saved results.

The screenshot displays the AI4Green Retrosynthesis web interface. At the top, there are navigation tabs for 'Compounds', 'Reactions', 'Routes', and 'Saved Results'. The main area is titled 'Retrosynthesis' and features a search bar with the chemical formula O=C1c2ccc(O)cc2c1 and a 'New Retrosynthesis' button. Below the search bar is an 'Interactive Retrosynthesis Display' showing a hierarchical reaction tree. The root node is a complex molecule, which branches into two intermediate nodes, and these further branch into four final product nodes. The final products are: 2-hydroxypyridine, 2-chloropyridine, 2-aminopyridine, and 2-pyridone. A 'Save To Workbook' button is visible in the top right of the interface. On the left side, there is a 'Saved Results' section with a 'Development Workbook' dropdown and a 'Saved results list' containing a 'Test Retrosynthesis' entry with a thumbnail image of a chemical structure and a 'Reload' button. At the bottom, there are references: 'Retrosynthetic routes predicted with AI₂ynthFinder: a fast, robust and flexible open-source software for retrosynthetic planning. J. Cheminform. 2020, 12, 70 (2020)' and 'Reaction conditions predicted with: Using Machine Learning To Predict Suitable Conditions for Organic Reactions. ACS Cent. Sci. 2018, 4, 11, 1485-1476'.

As an alternative to using the retrosynthesis, a file can be uploaded with route details in the route tab using the same format as found in the example file. This will display and assess the sustainability of the route in the same method.

8. Further Help

Our Help page is accessible from the Navigation Bar. Please see here for useful guides and video tutorials. You can also send any queries to admin@ai4green.app and a member of the team will respond to your request.

The screenshot shows the AI4Green Documentation & Help page. At the top, there is a navigation bar with links for Home, Demo, Solvents, Retrosynthesis, and Workgroup, along with a search icon. On the right side of the navigation bar, there are links for About AI4Green, Help, and a user profile for User 1. The main content area is titled "AI4Green Documentation & Help" and "Video Tutorials". It includes a paragraph stating that several video tutorials are available to explain Workgroups & Workbooks, the Reaction Constructor, and the Solvent Guide. Below this is a video player showing a thumbnail for "AI4Green Reaction Constructor 1.4". Underneath the video player, there is a "Watch on YouTube" button. The "User Guides" section contains four buttons: "Quickstart Guide", "User Guide", "Marvin JS Help Page", and "Reaction Builder Tutorial 3B". Below the user guides, there are links for "Click here to view the privacy notice" and "Click here to view the hazard disclaimer". At the bottom of the main content area, there is a "GitHub Repository" button and a contact email: "For further help, queries or suggestions please feel free to contact us: ai4green@nottingham.ac.uk". The footer of the page contains the AI4Green logo, links for Hazard Disclaimer, Privacy Notice, Twitter, and GitHub, and a note that hazard data is sourced from ECHA references on PubChem.