AI4Green

Version 1.6 User Guide

August 2024

Supported by

The University of Nottingham

Royal Academy of Engineering

Contents

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.

Users are researchers with accounts on AI4Green

Workgroups are collections of **Users**

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

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

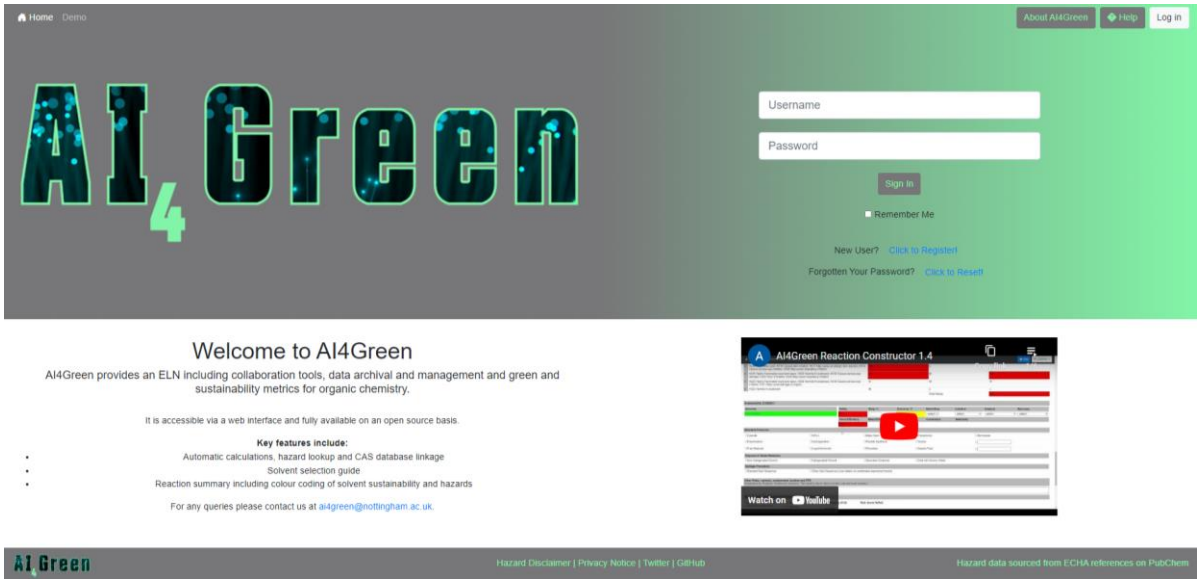
Reactions contain experimental information obtained from the lab

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.

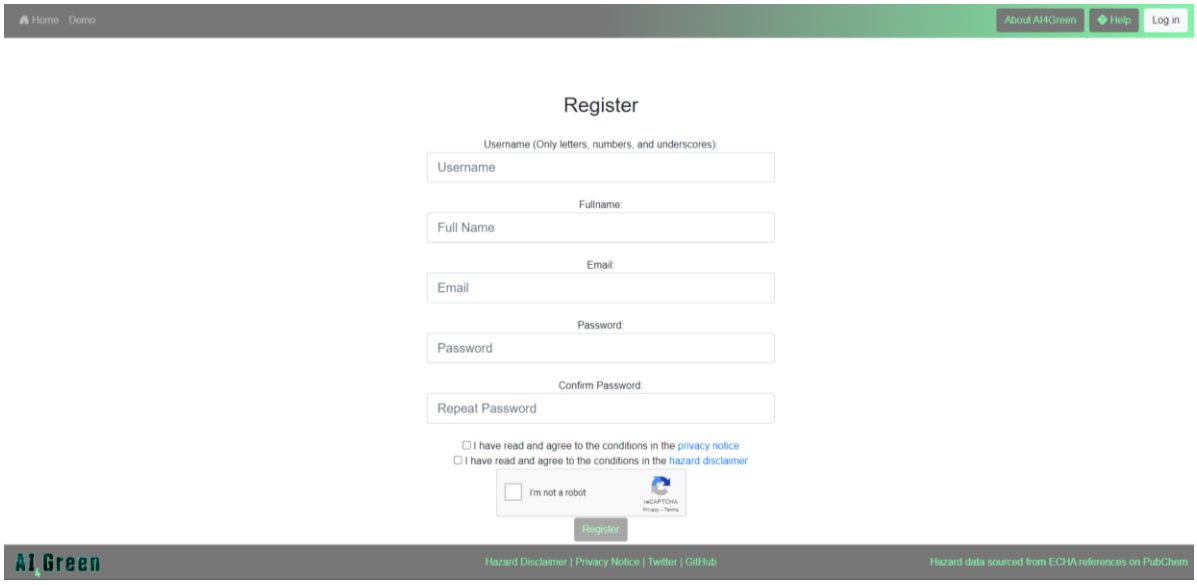
The landing page will prompt you to log in or register if you do not have an account. Our YouTube channel provides some excellent quick start videos, which can be accessed from this page.



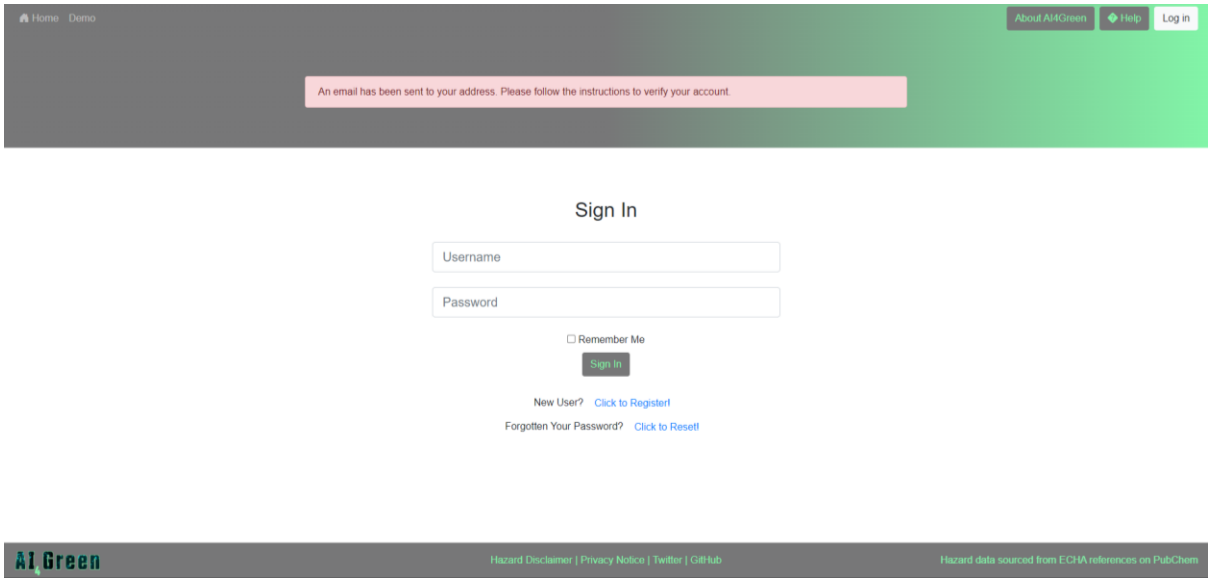
3.1. Registering as a New User

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.

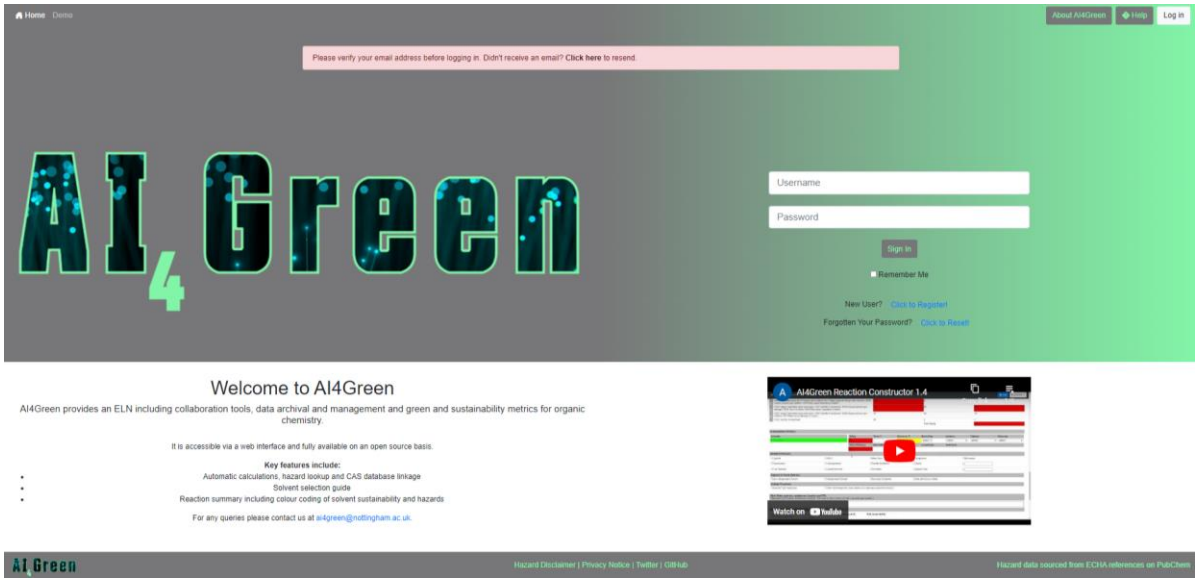
Click to Register! will direct you to the registration page, which will prompt you to enter a username, your full name, email address and a unique password. Please note that only letters, numbers and underscores are permitted in your username. You will also have to agree to our privacy policy and hazard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



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.



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.

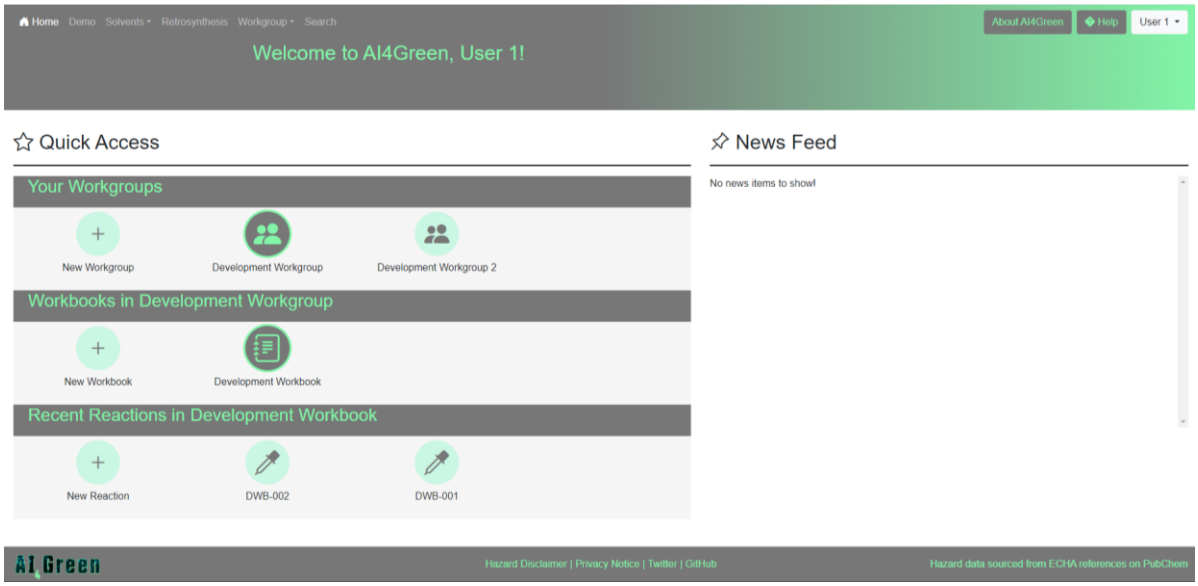


3.2. The Home Page

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.

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.

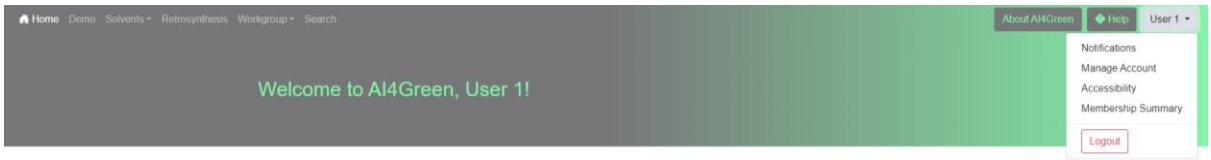


Any member of a Workbook can create a reaction with the “New Reaction” icon. Selecting any Reaction icon loads the corresponding Reaction page.

3.3. The Navigation Bar

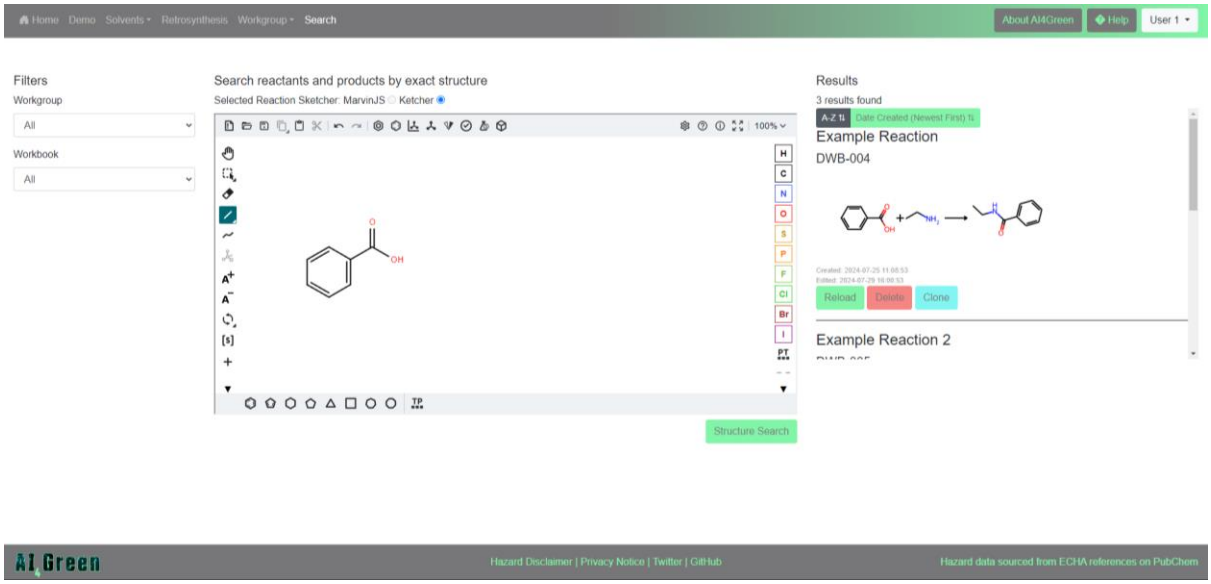
The top navigation bar is the same on any page in AI4Green, and the left-hand side provides quick links to the home page, demo reaction constructor, Solvent Guide or Solvent Surfer (under the Solvents Tab), Retrosynthesis tool, Workgroup Management page (under Workgroups tab) and the Search function.

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.



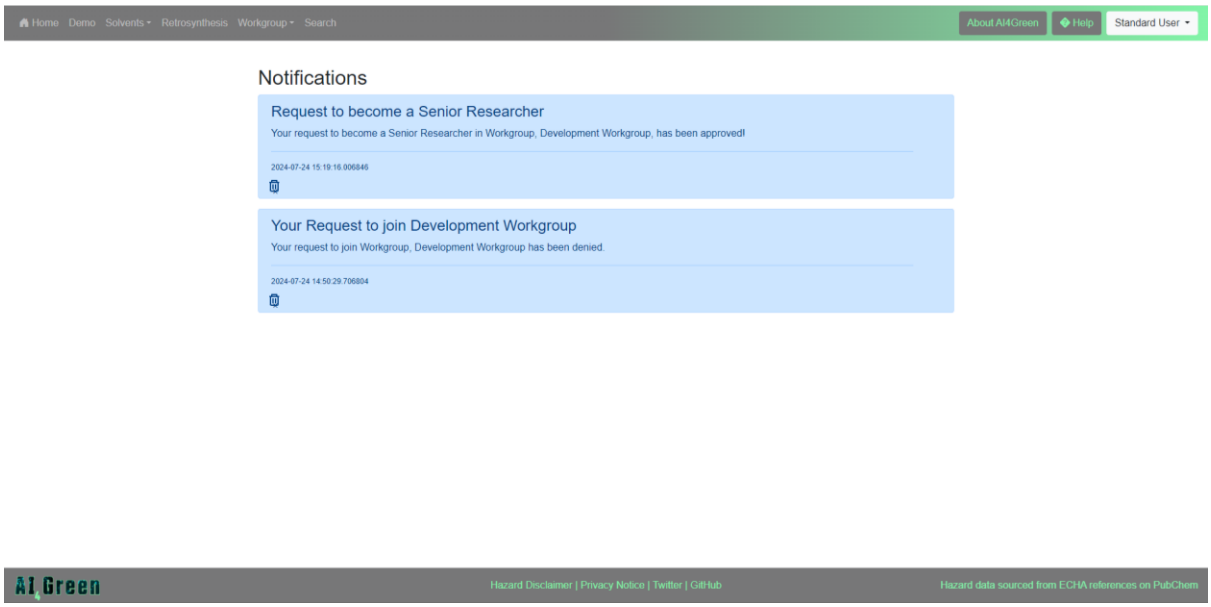
3.3.1. Search

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.



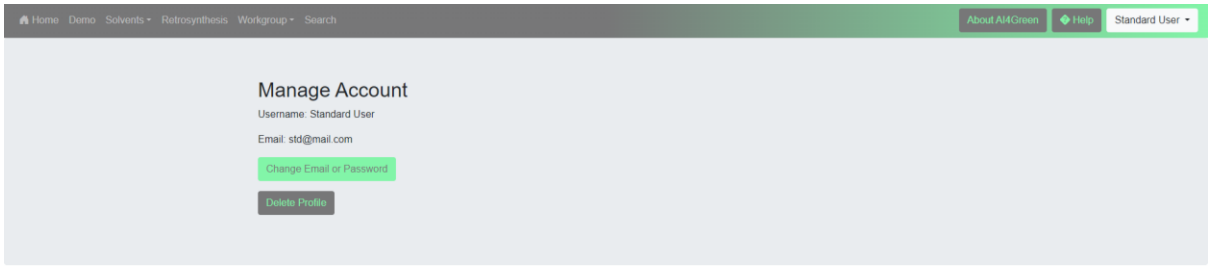
3.3.2. Notifications

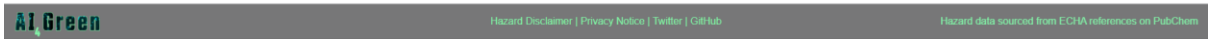
Your notifications are accessible from the User dropdown menu on the right-hand side of the Navigation bar. These are used to keep you up to date with any requests you have made. These include being added to a Workgroup or Workbook, changing user status or exporting data. You will receive an email when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



3.3.3. Manage Account

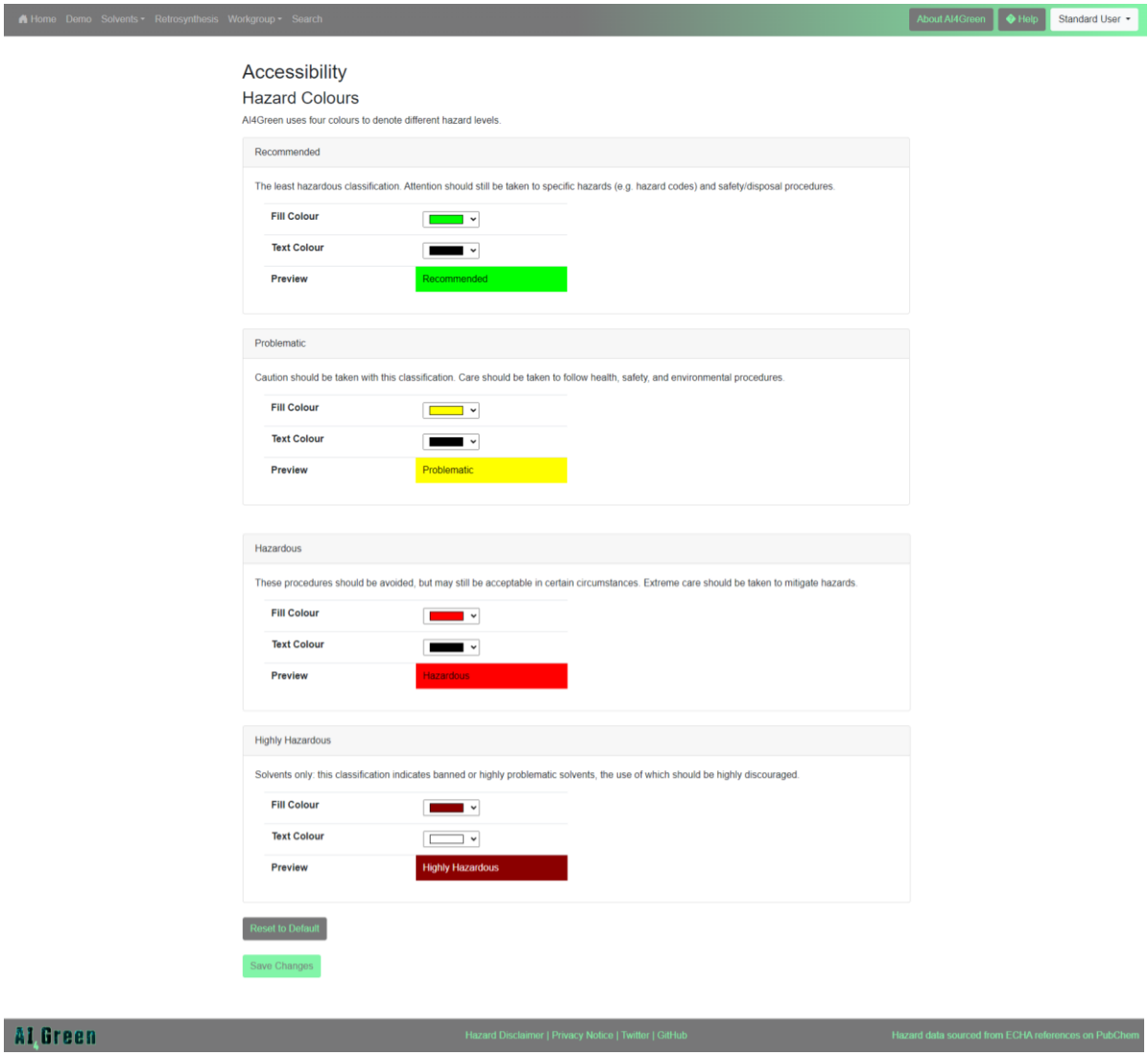
You can manage your account from the User dropdown on the right-hand side of the Navigation bar. This lets you change your email, change your password, or delete your account.





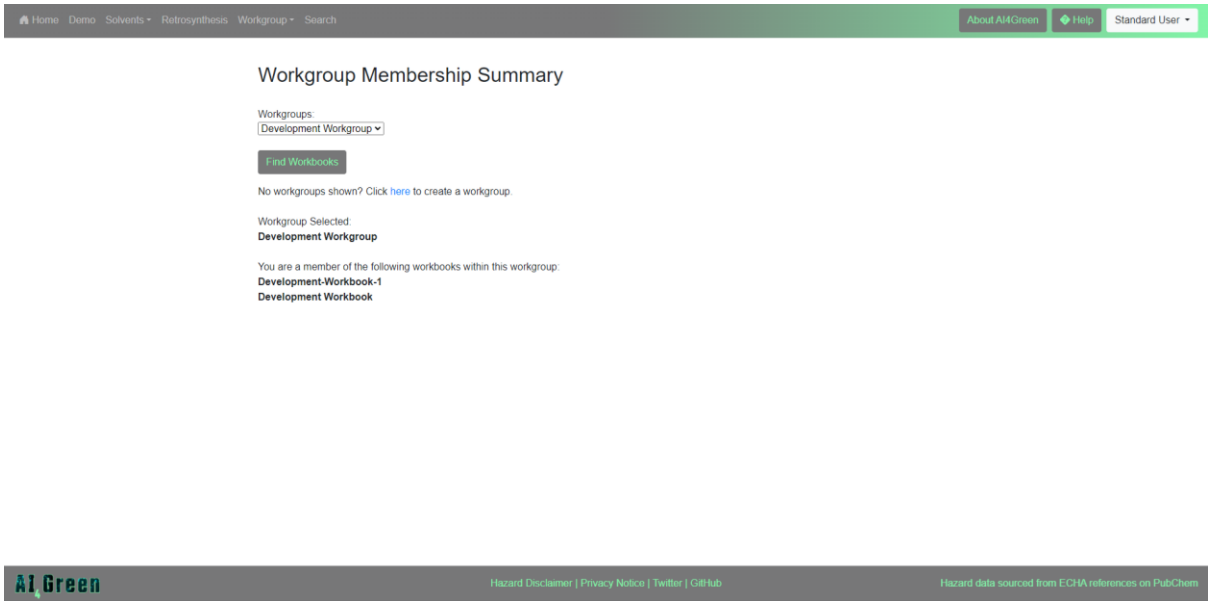
3.3.4. Accessibility

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.



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.


Home
Demo
Solvents
Retrosynthesis
Workgroup
Search
About AI4Green
Help
Standard User
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
AI4Green
Hazard Disclaimer | Privacy Notice | Twitter | GitHub
Hazard data sourced from ECHA references on PubChem

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.

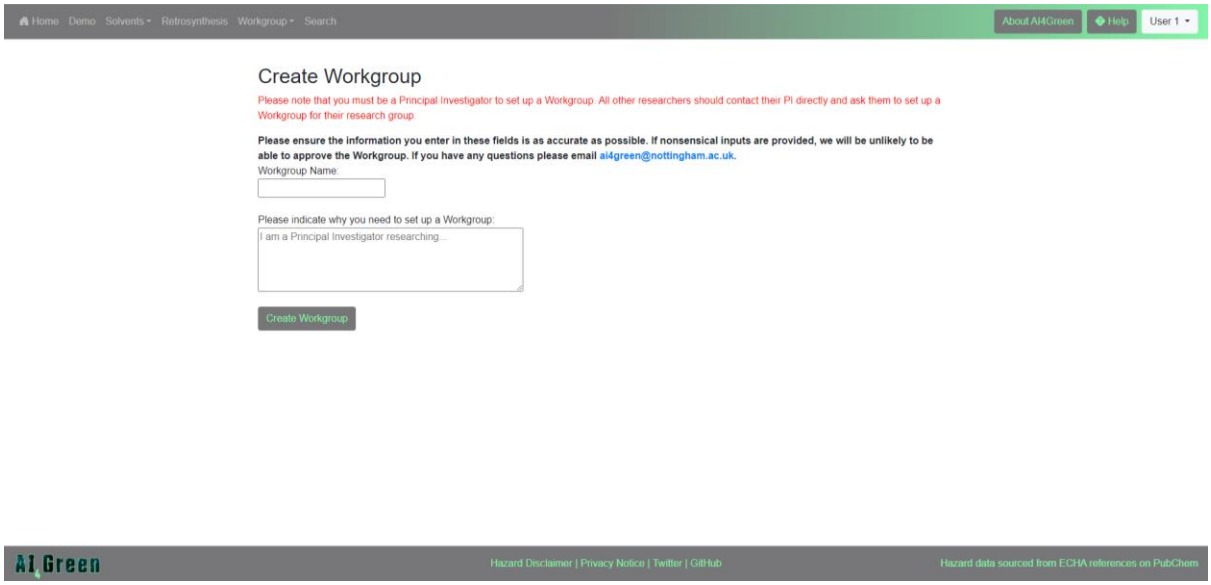
4.1.3. Standard Member

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

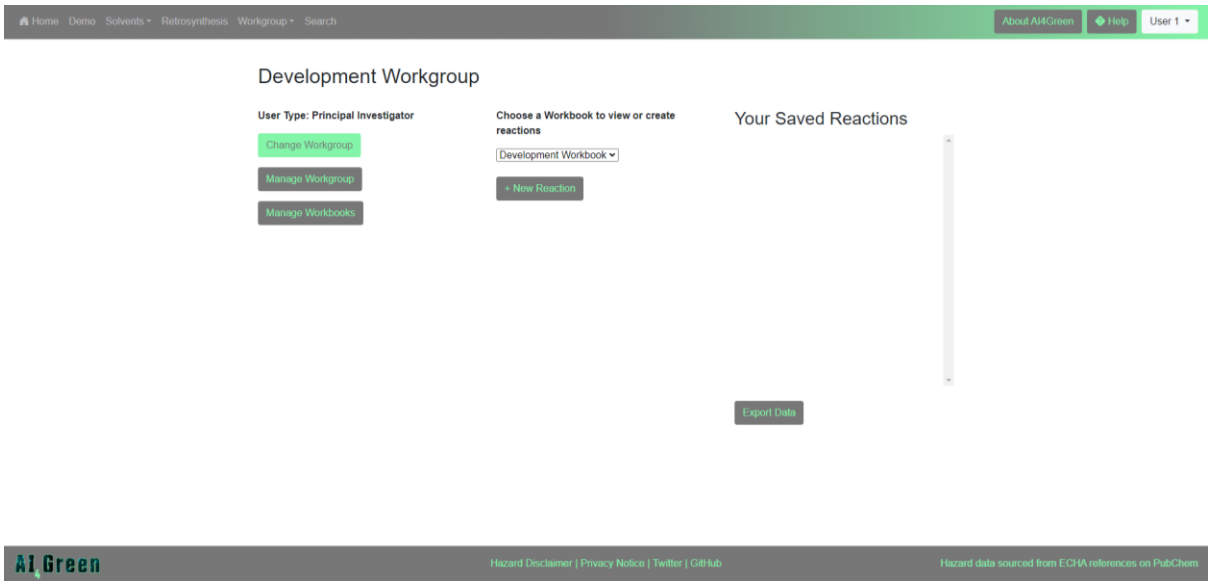
Workgroups can be created by clicking on the “New Workgroup” icon in the Quick Access panel on the home page. This navigates you to the “Create Workgroup” page, which prompts you to enter a name for your Workgroup and a brief explanation of your research. Each Workgroup must be approved by our admin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



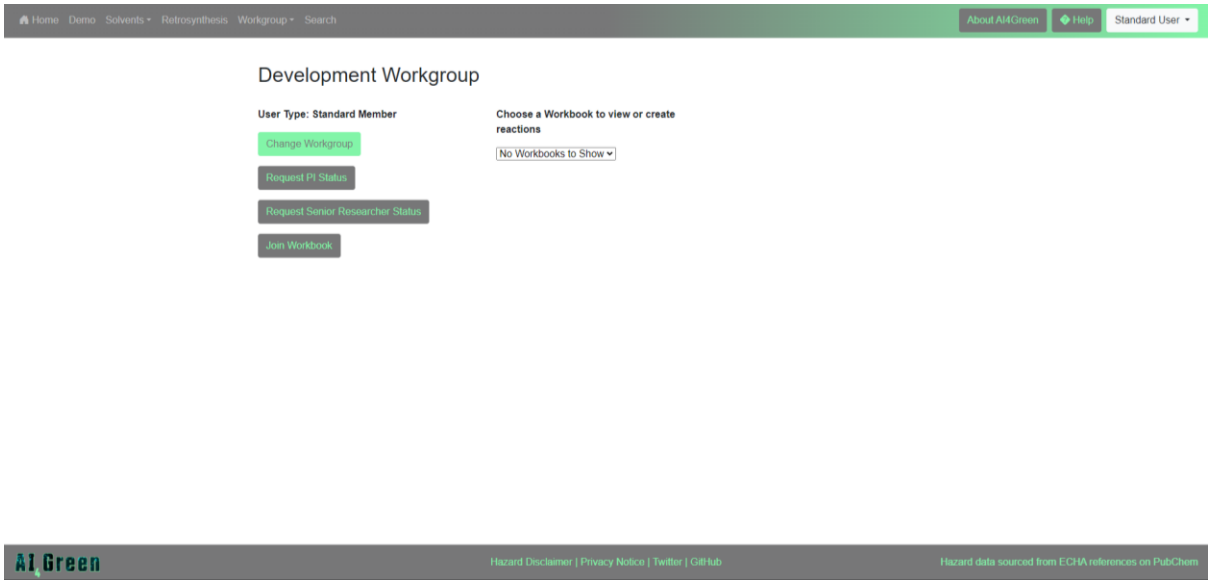
4.3. The Workgroup Page

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.



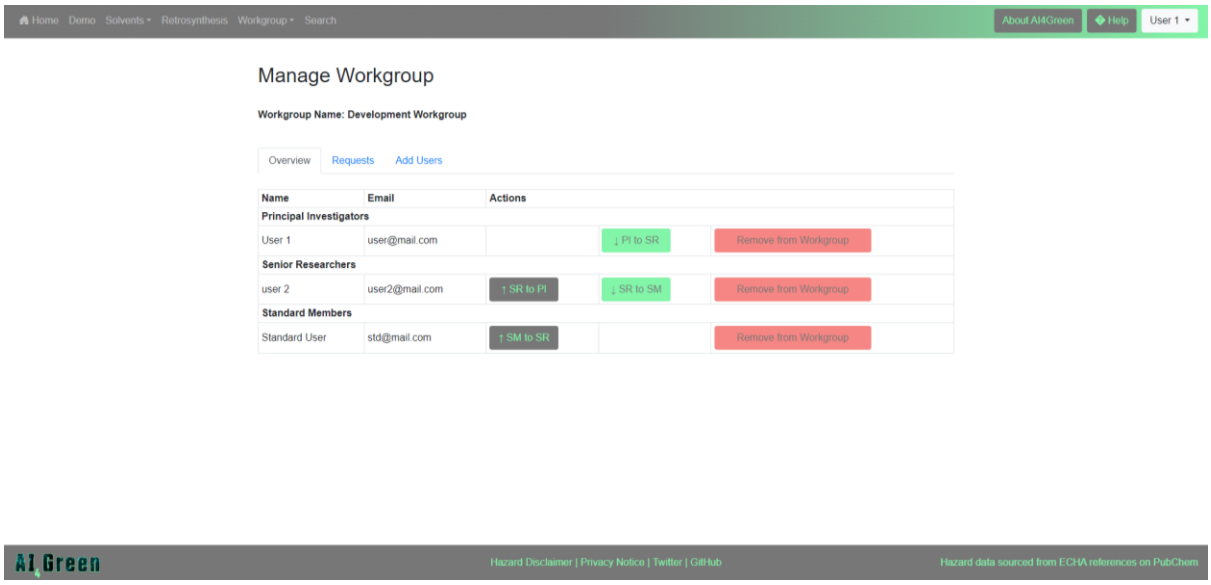
From this page, Senior Researchers and Standard Members can request a change of status. See below for an example for a Standard Member. Senior Researchers and Standard Members can also request to join a Workbook in the Workgroup using the "Join Workgroup" button.



4.4. Managing Workgroups

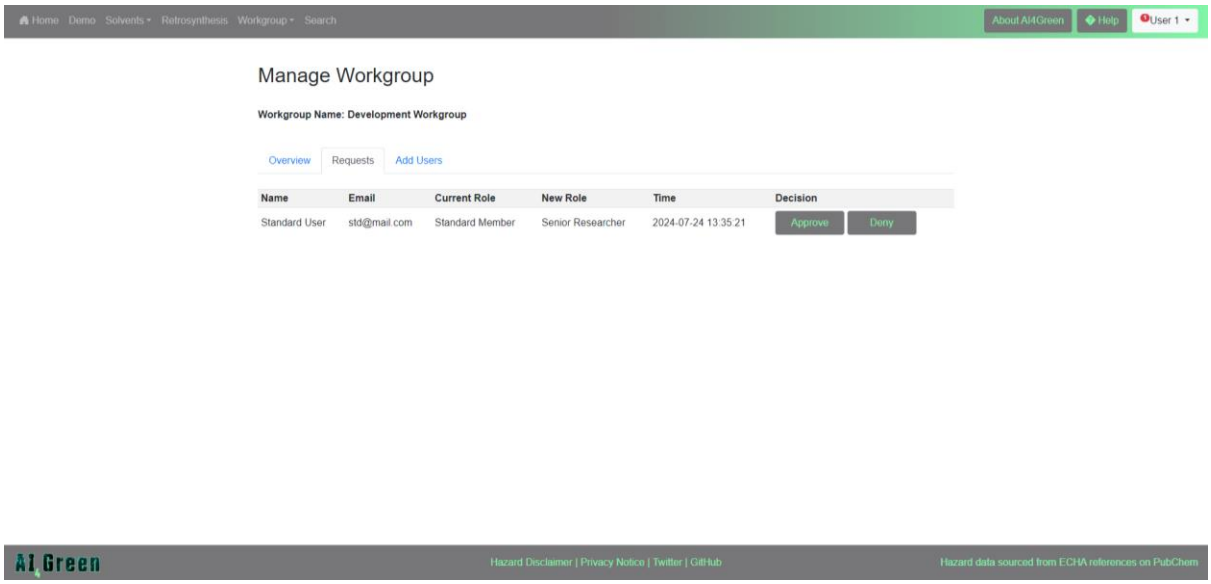
4.4.1. Overview

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.



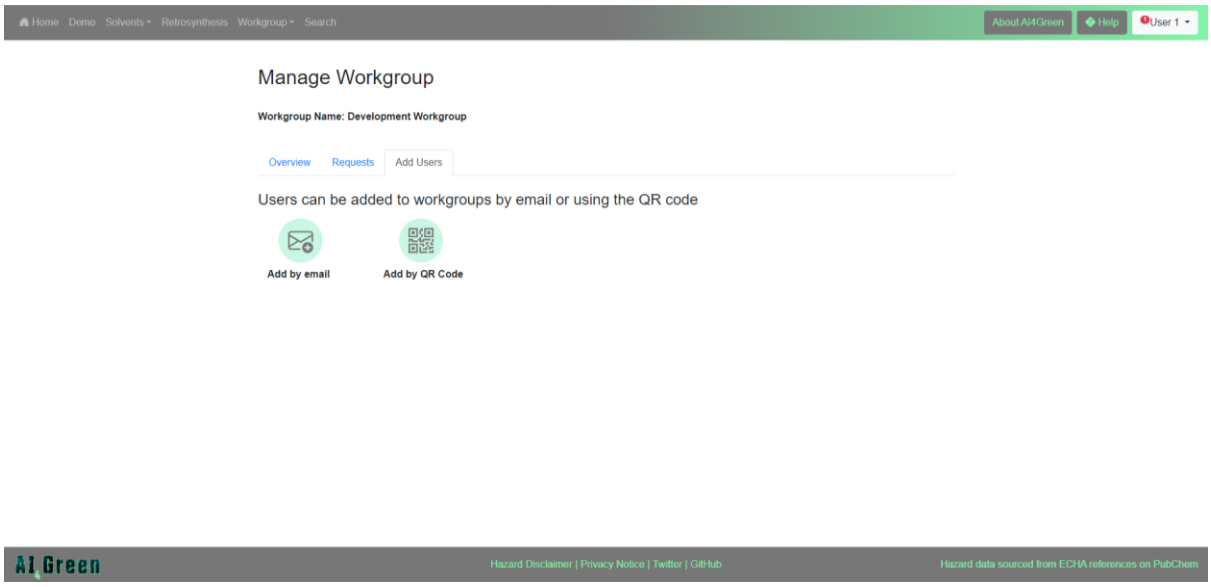
4.4.2. Requests

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.

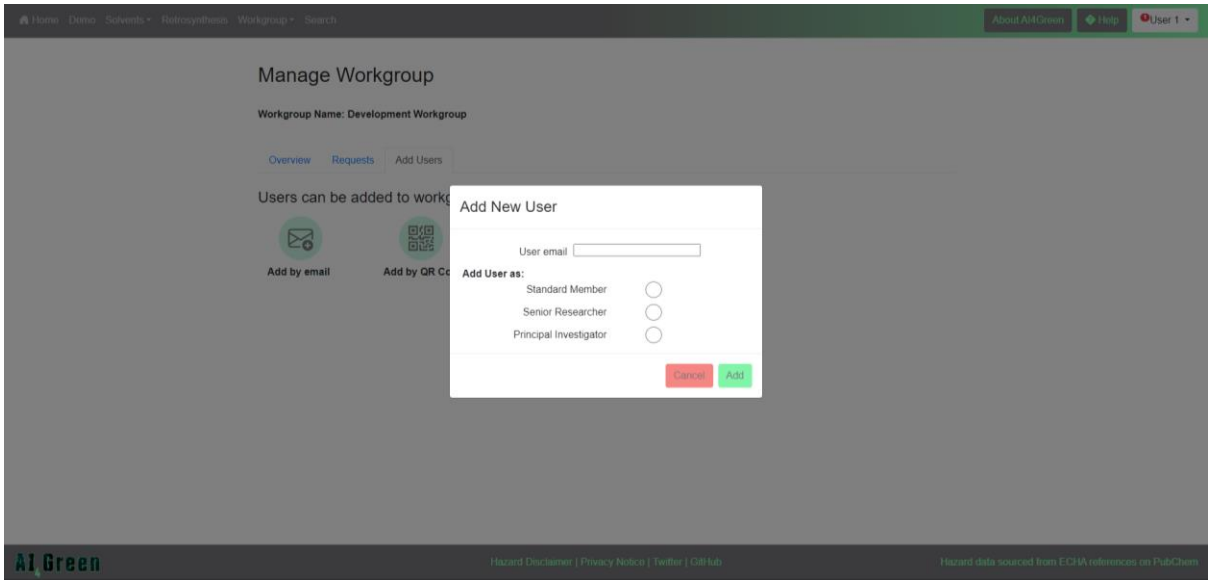


4.4.3. Add Users

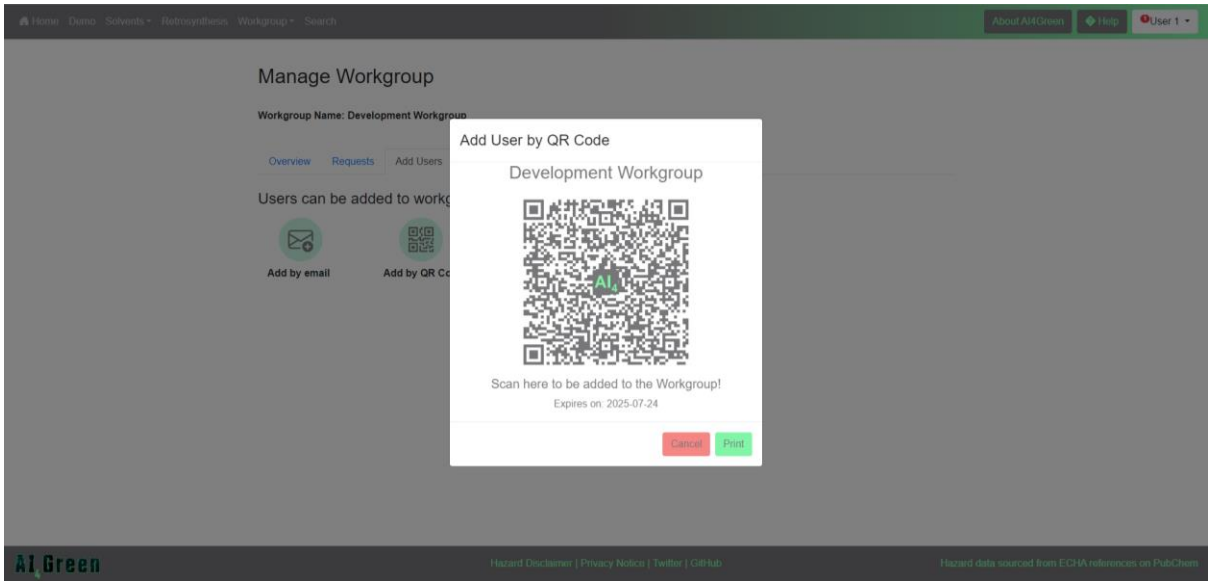
Adding users to Workgroups has changed from previous versions. There are now two ways to add users to a Workgroup, via email or QR code.



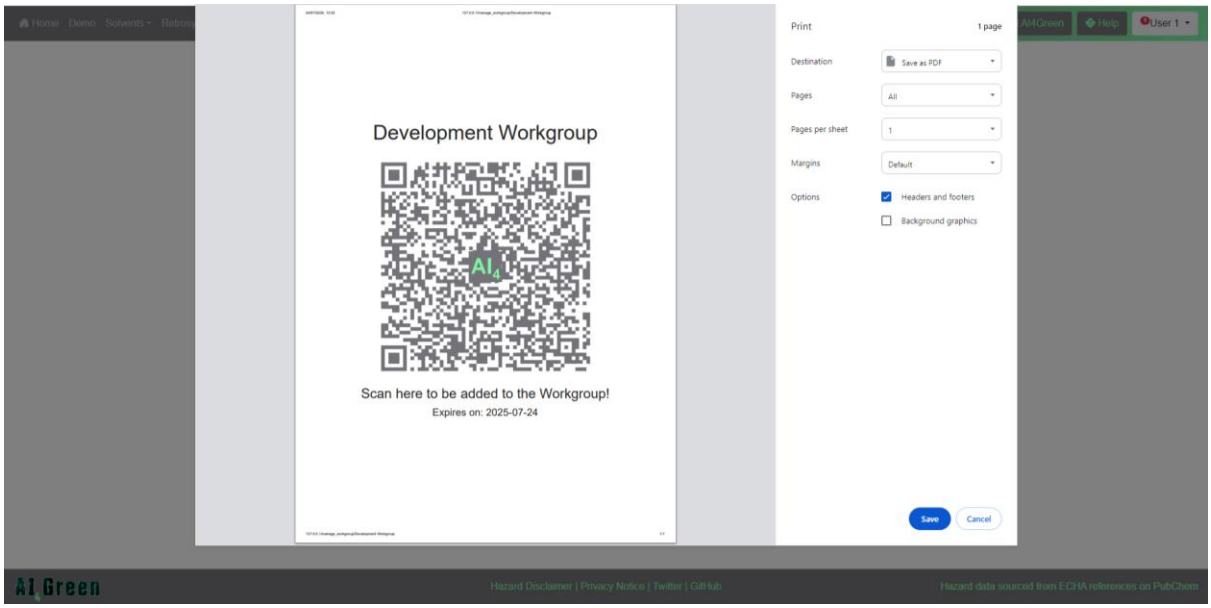
Principal Investigators can add users by their registered AI4Green email address by clicking on the “Add by email” icon. This will prompt you to enter the email address of the user you want to add and to select a membership level for the new user. This will send a request to the added user and will need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



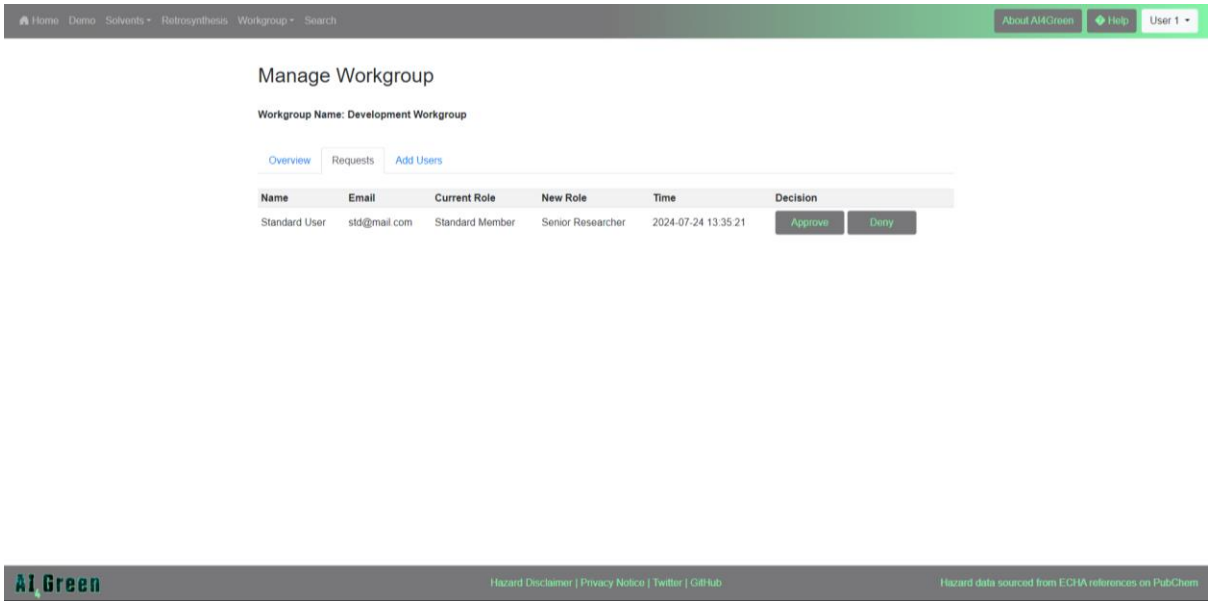
Alternatively, users can be added by scanning a generated Workgroup QR code. This provides an alternative option and allows for the addition of multiple users without having to enter each individual email, which can be time consuming. Instead, QR codes can be circulated to users who would like to join 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.



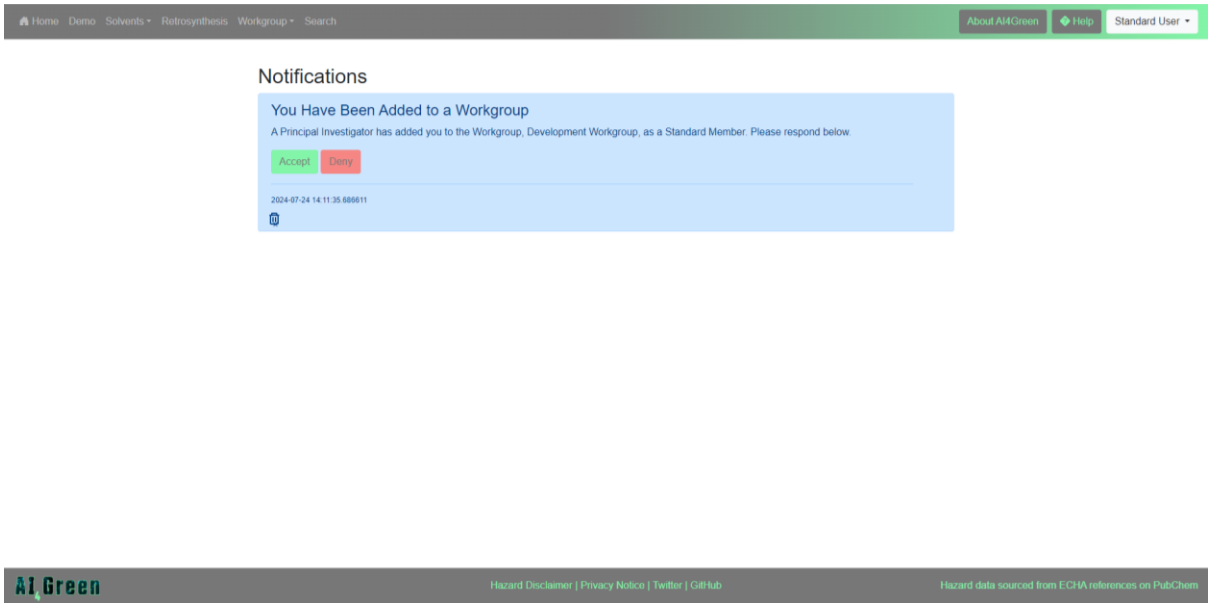
When a user scans a QR code, a membership request is sent to the Principal Investigator of the Workgroup and their approval is needed before the user is added. This provides an extra layer of security. You will receive a Notification about this request, which you can then view under the request tab.



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.

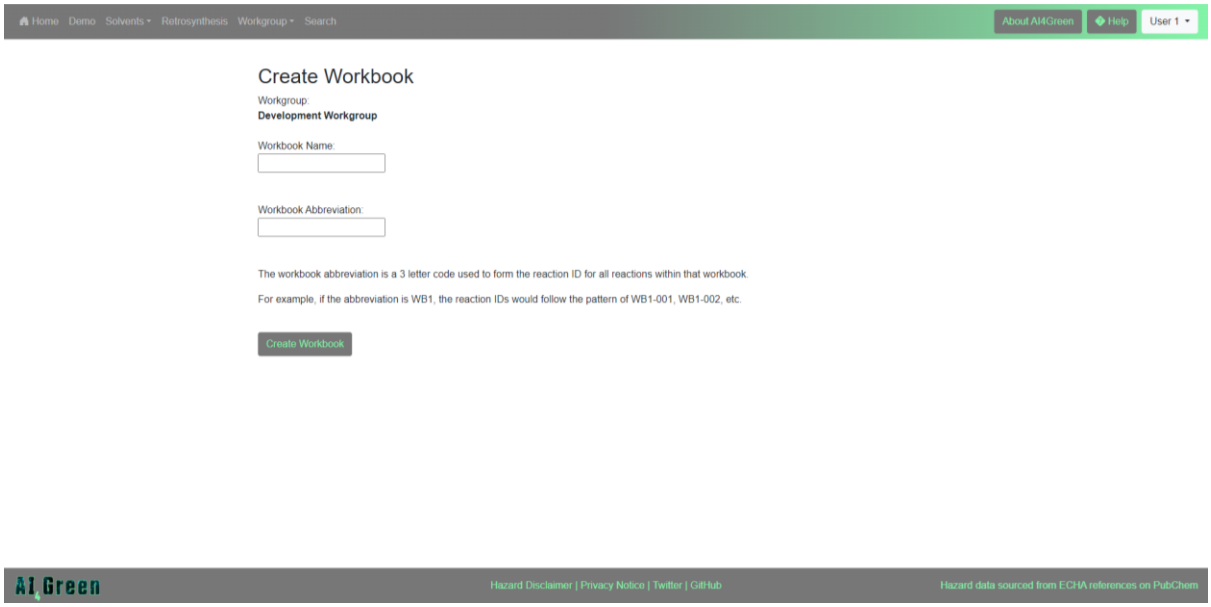


5. Workbooks

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

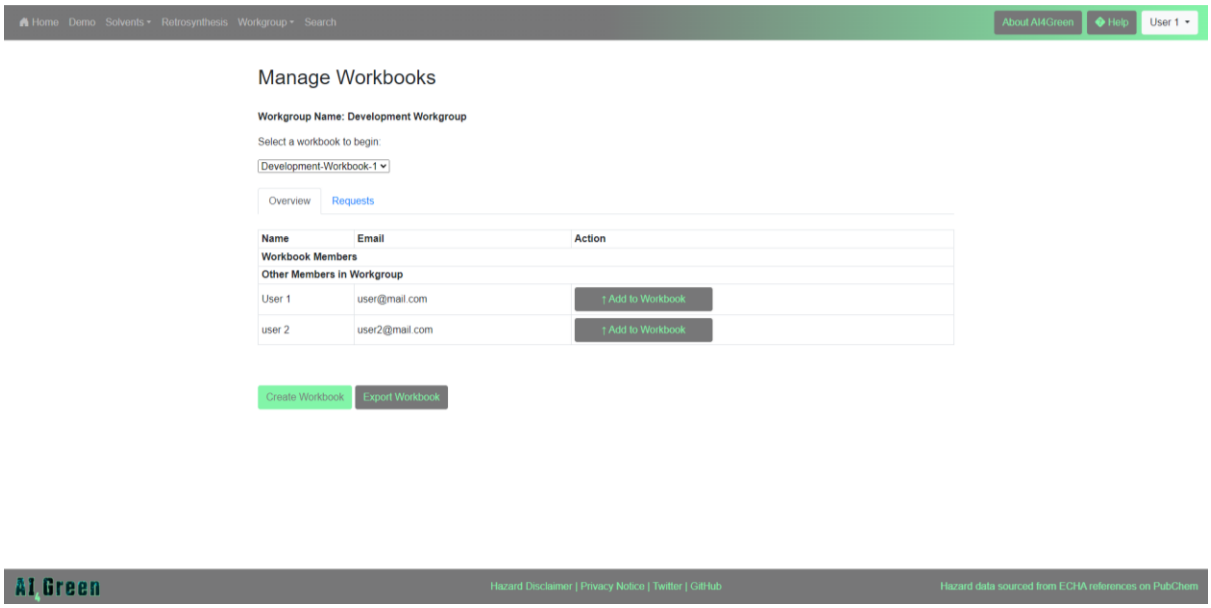
Workbooks can be created by Senior Researchers or Principal Investigators and can be done either from the Quick Access panel on the home page or from the Manage Workbooks page. When creating a new Workbook, you will be prompted to enter a Workbook name and 3 letter abbreviation for your Workbook – this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



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.

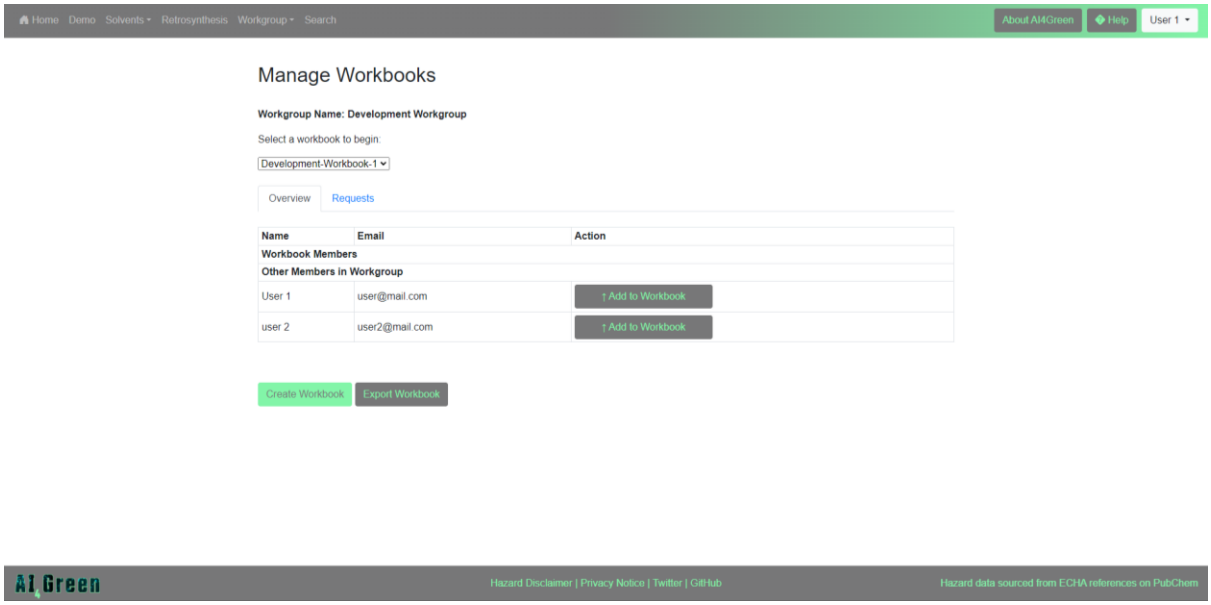
5.2. Managing Workbooks

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.



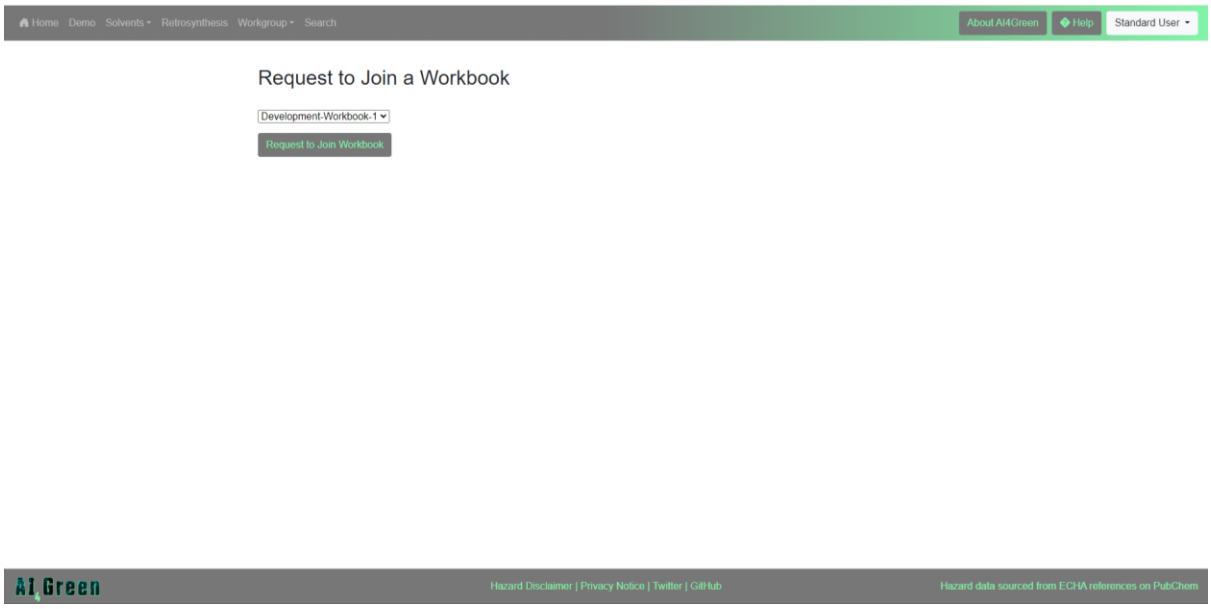
Selecting a Workbook from the dropdown allows you to manage that Workbook. Users in the Workgroup can be added to the Workbook at any time. All Principal Investigators and Senior Researchers can manage all Workbooks within a Workgroup.

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.



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.



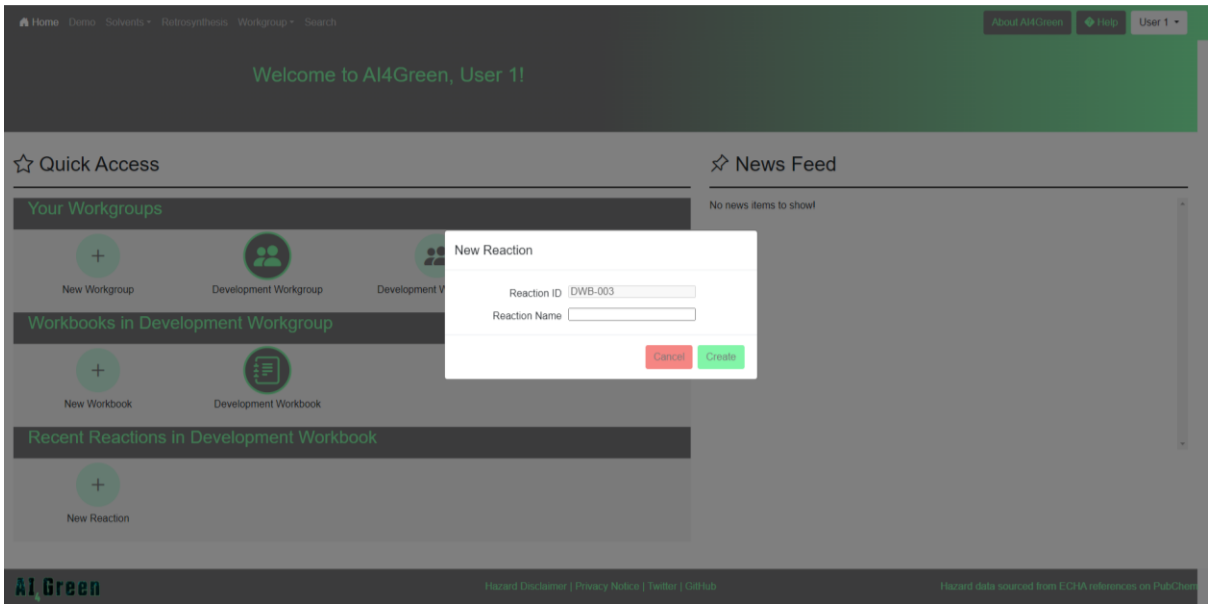
Principal Investigators and Senior Researchers have access to the Manage Workbooks page, so can be added to Workbooks from here.

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

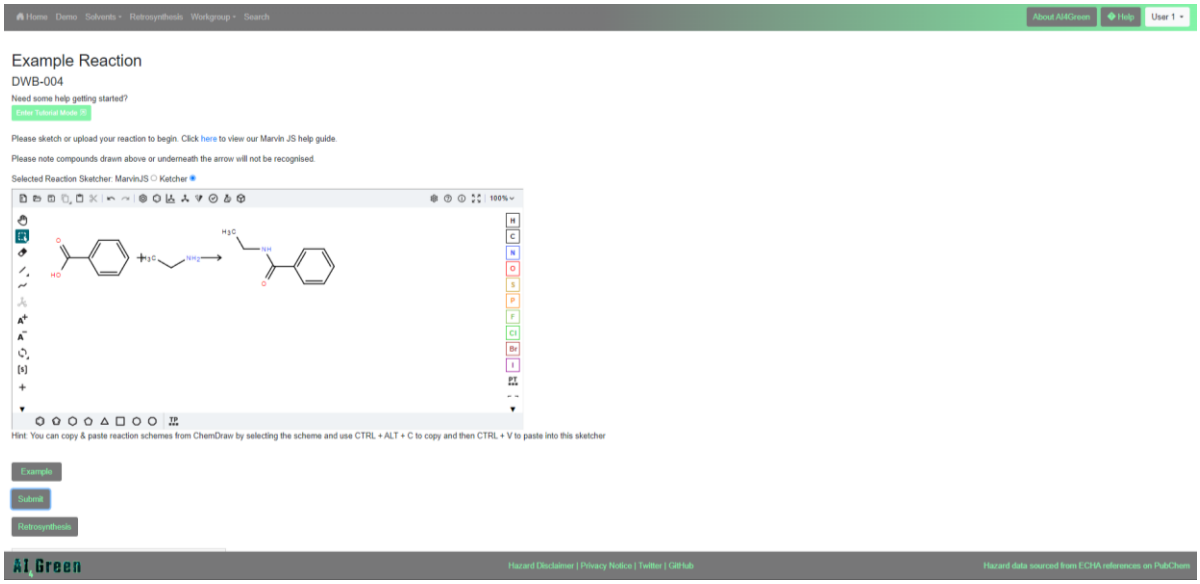
The Reaction Constructor allows you to include all the necessary reaction data needed to carry out synthetic organic chemistry. This section will discuss in detail each of the sections of the reaction constructor. All changes made to Reactions are saved automatically. For a tutorial on how to use the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

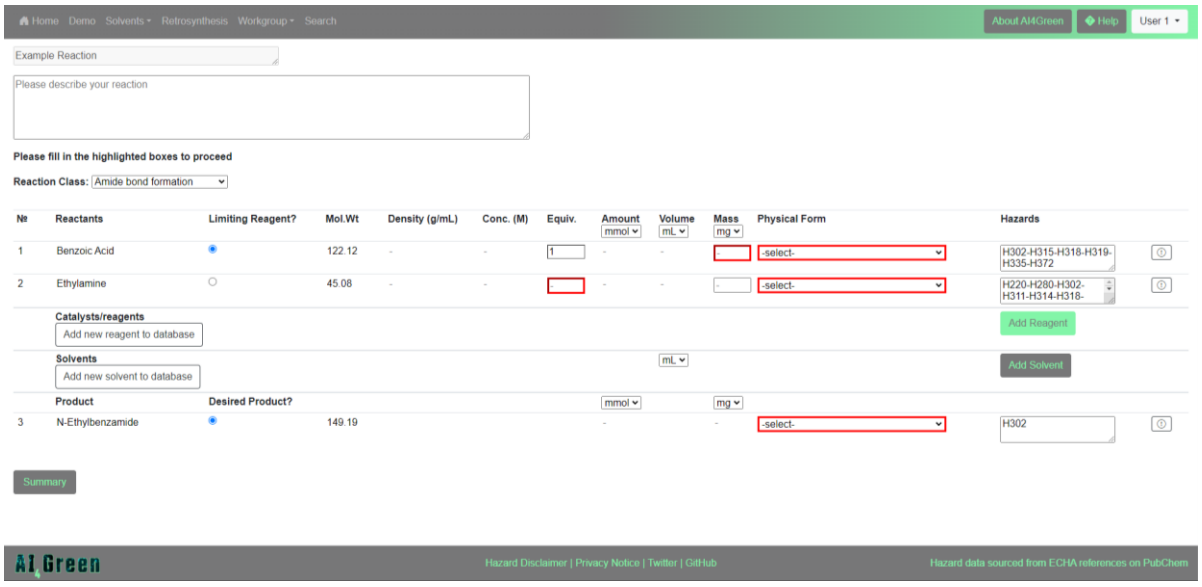


5.5.2. The Reaction Table

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.



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.

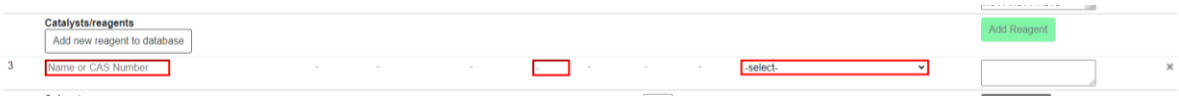
Reagents and solvents must be added separately using the “Add Reagent” and “Add Solvent” buttons.

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.



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.

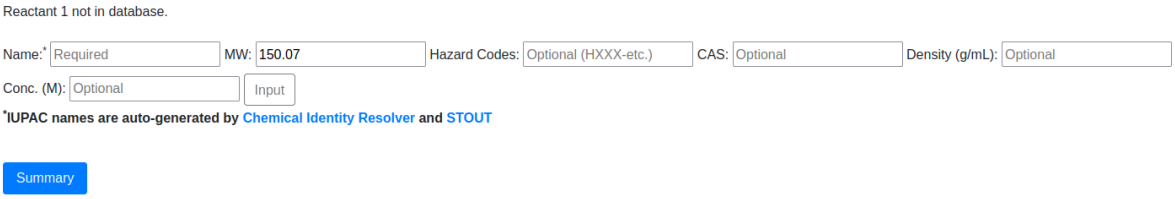
The volume and physical form are required here.

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.

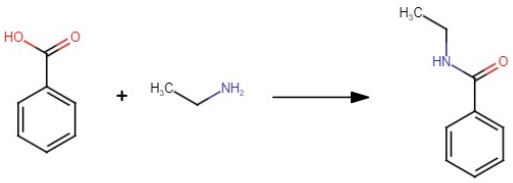
To add a novel compound, you will be prompted to provide as much information as possible regarding this compound. Once done, click ‘Input’.



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.



№	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
	Solvents						**Volume (mL)**	
5	Ethyl acetate						2	
	Product	**Mol.Wt**	**Theoretical Yield (mg)**		**Unreacted**	**Product Mass (mg)**	**% Yield**	
6	N-Ethylbenzamide	149.19	122		-	-		

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

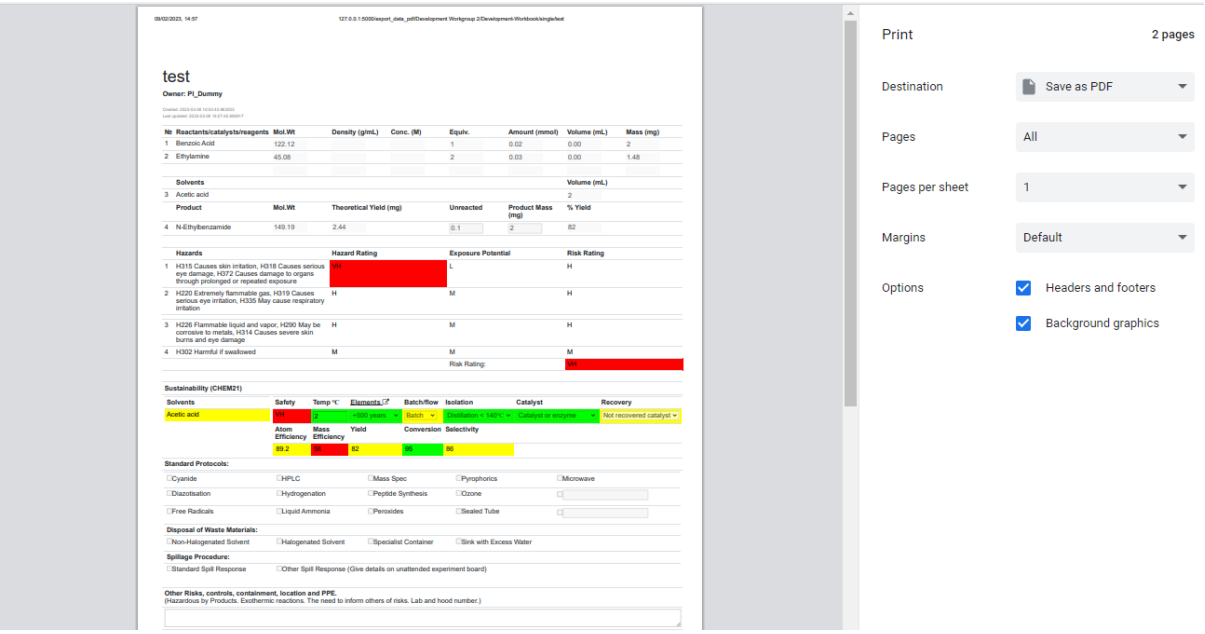
There is also some additional safety and sustainability information to enter to calculate the green metrics for your reaction. This is where you can record the temperature, the reactor type (batch/flow), isolation method, stoichiometry and catalyst recovery steps. These all give a sustainability score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

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.

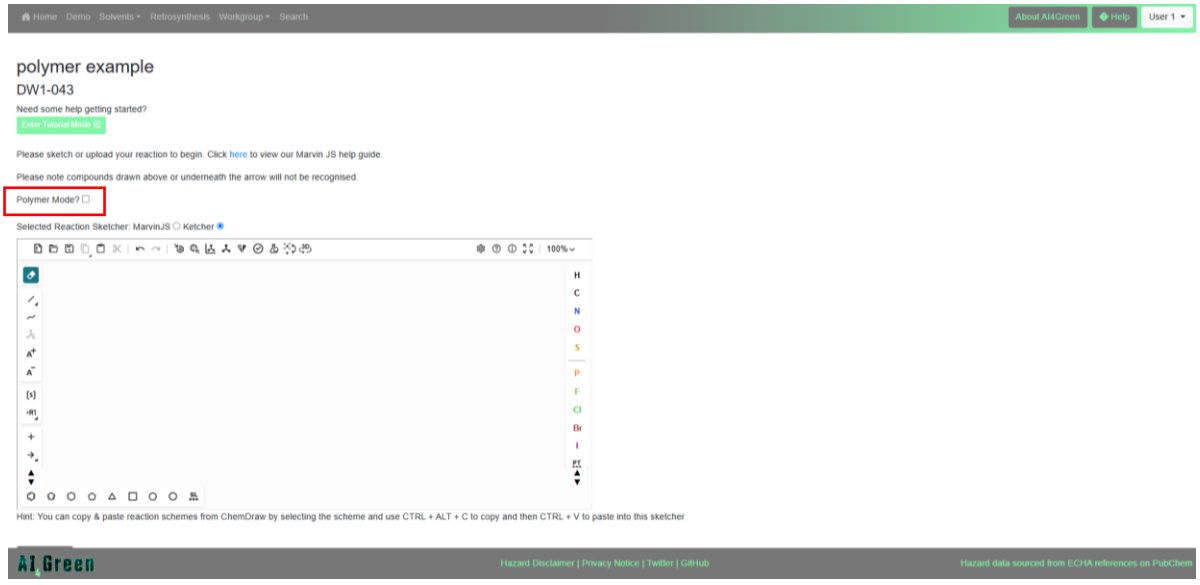
This printout can be taken into the lab and placed near the reaction to act as a reference for the COSHH + H&S data for the reaction. If you are using this as a risk assessment in the laboratory, it MUST be signed off by both you and your supervisor.



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.



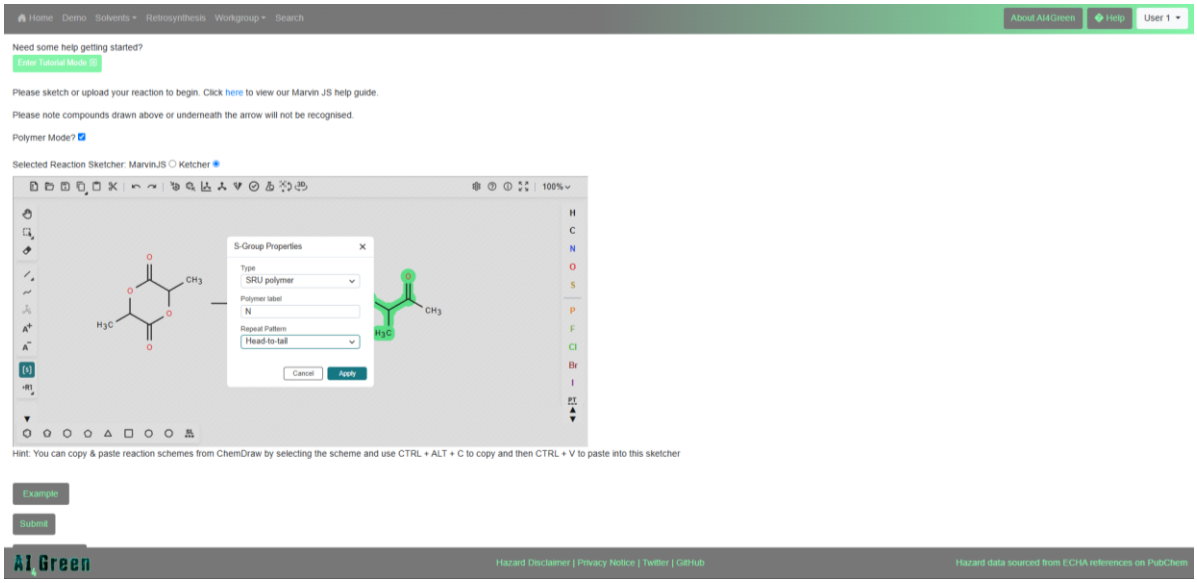
There are a few differences between polymer mode and the standard reaction constructor. These include drawing structures, the reaction table and the summary table.

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.

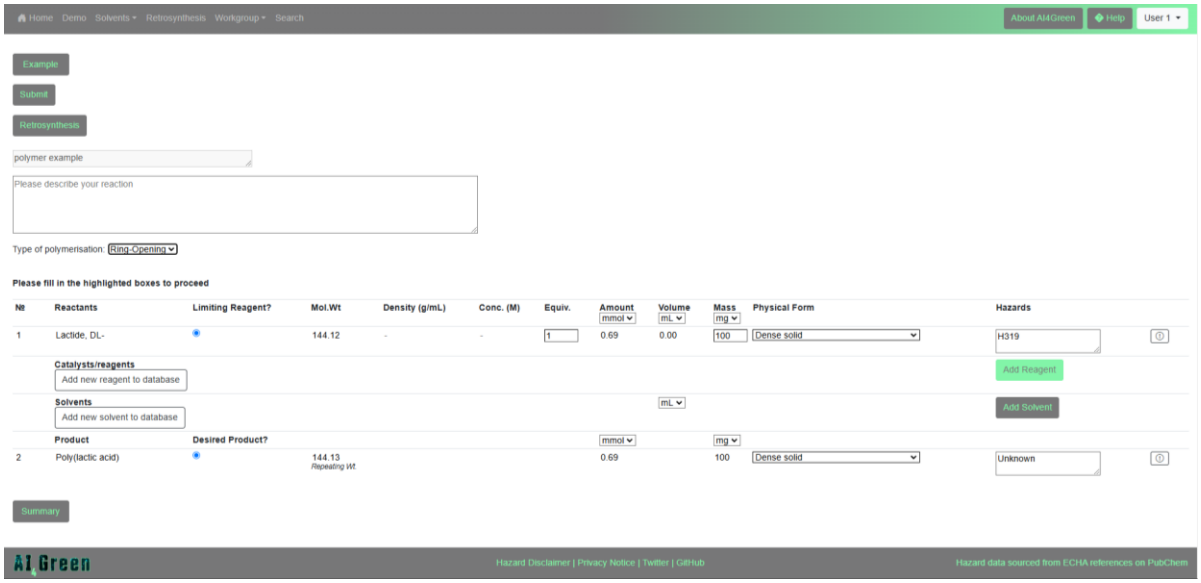
This tool will bring up the “S-Group properties” dialogue box, and polymers can be marked by selected “SRU Polymer” from the Type dropdown. SRU stands for Structural Repeating Unit. Selecting SRU polymer encloses the highlighted atoms within square brackets, which can be given a label by filling in the “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.



The Reaction Table

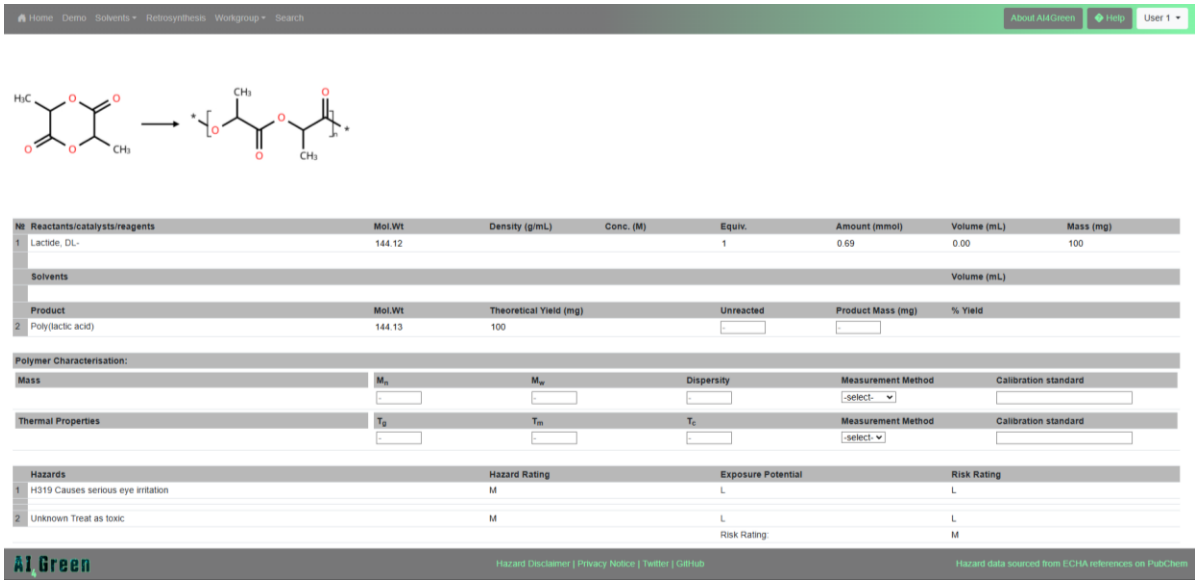
The reaction table is mostly the same as the standard reaction constructor, though the molecular weight is provided for the repeating unit only. A new drop down is also generated, in which you can specify the type of polymerisation.



The Summary Table

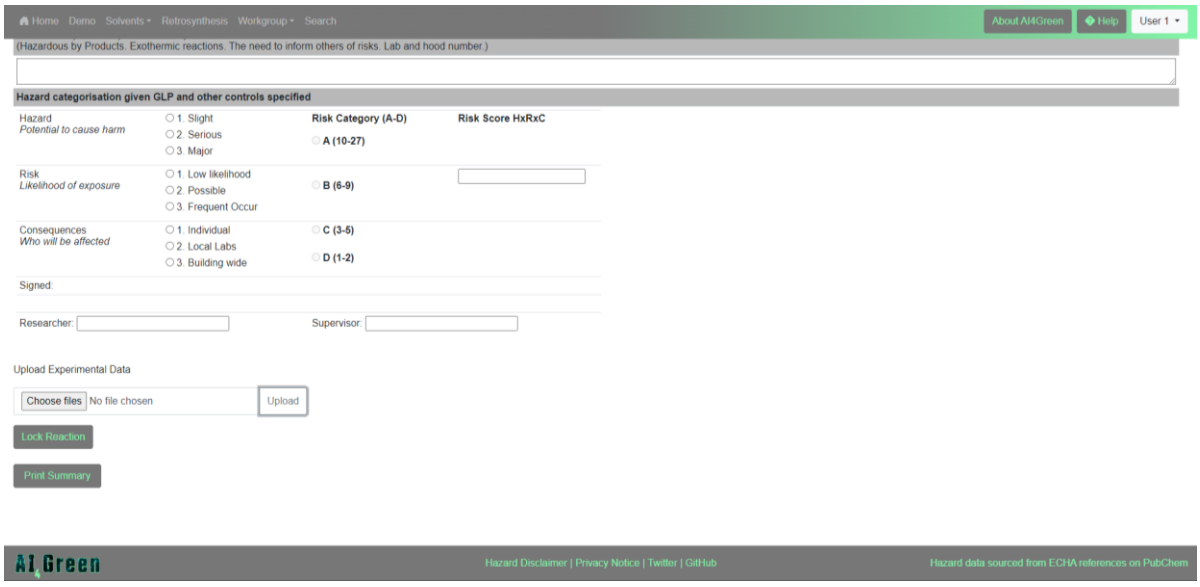
The summary table remains the same as the standard reaction summary, but the input fields for experimental data are different. The unreacted mass and percentage yield can still be recorded, but extra fields for the number-averaged and weight-averaged molecular weights,

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



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.



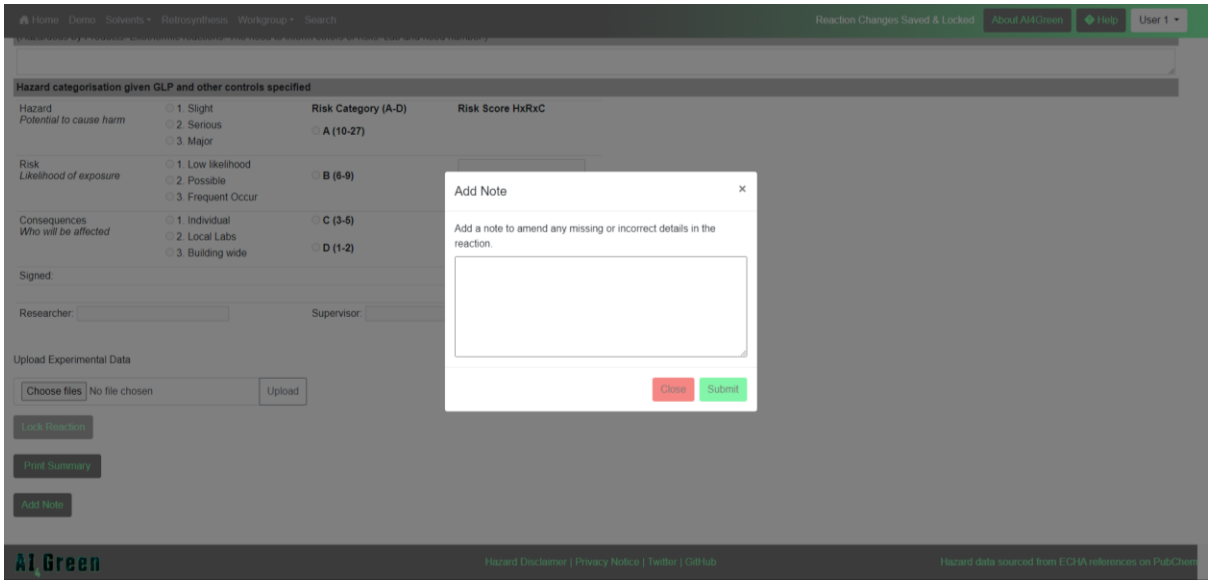
Only files with the following extensions can be added at this time:

.arw, cif, .cdf, .cdx, .csv, .D, .dat, .DTA, .dx, .fid, .gz, .jpg, .jdx, .jcamp, .mnova, .pdf, .pkl, .png, .pdb, .pssession, .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.

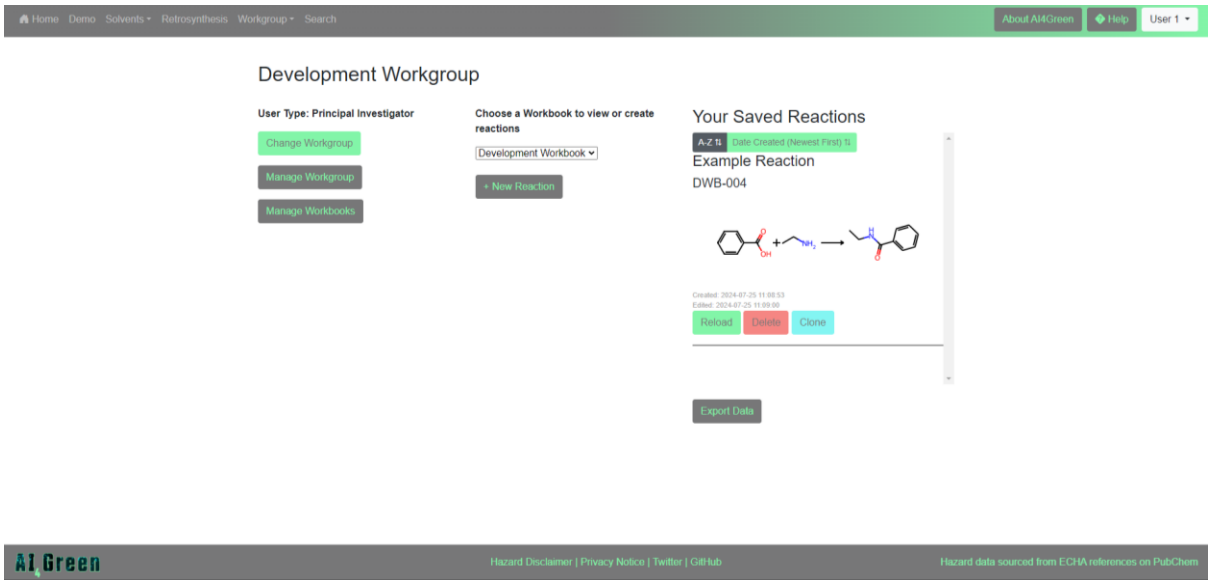


5.7. Saved Reactions

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.

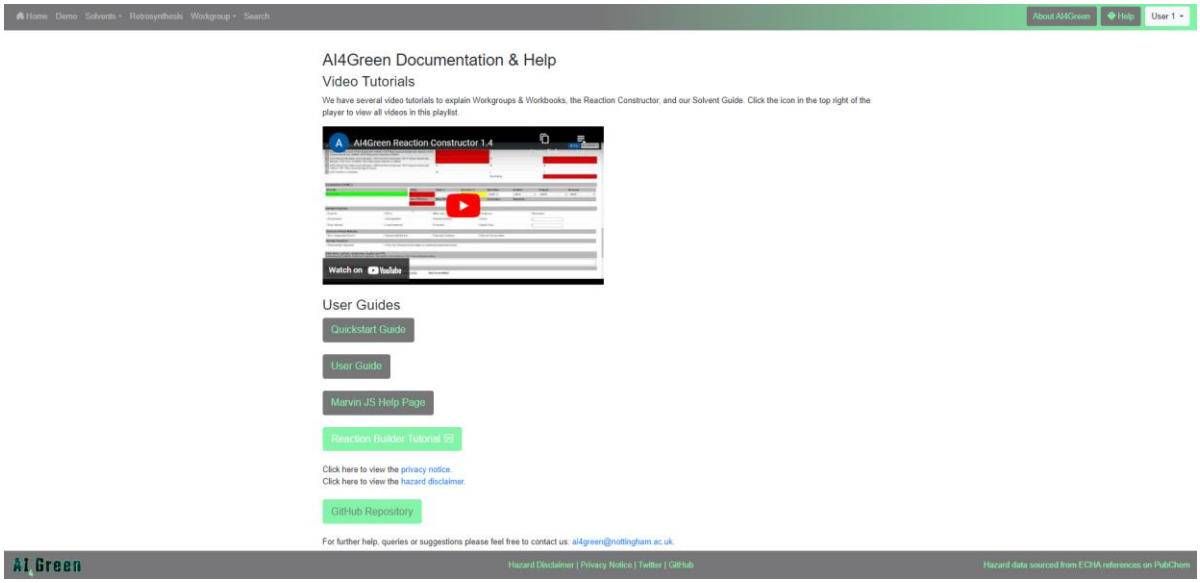
On the Workgroup page, users can view all Reactions in the workbook and order them either alphabetically or by date created. Each Reaction is summarised with its reaction scheme, the date of creation, whether the Reaction is locked and whether the Reaction contains any notes (amendments).

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.

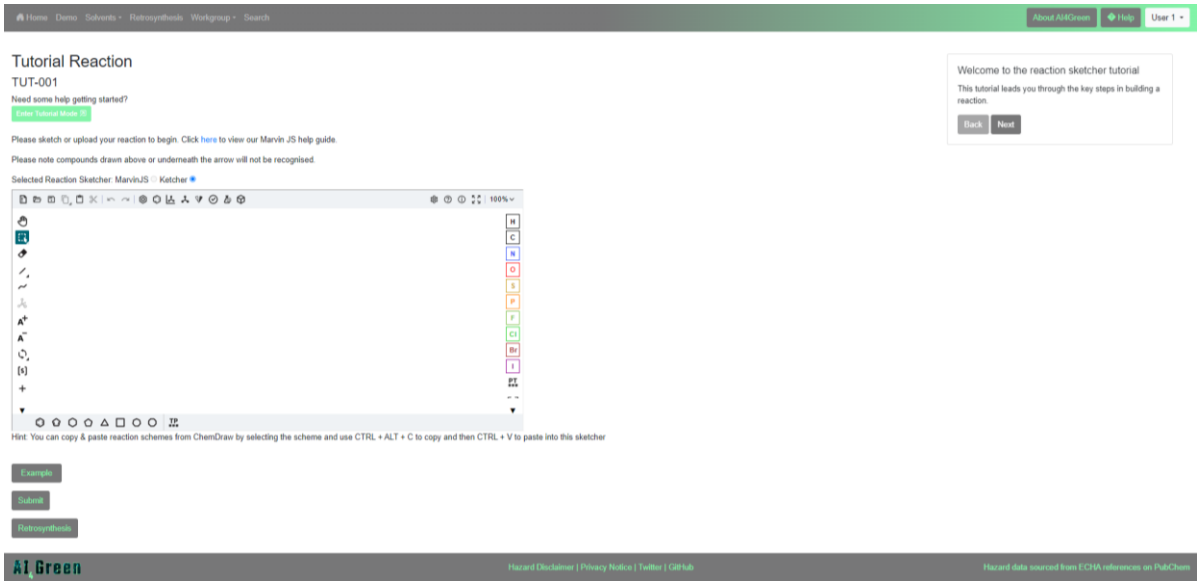


5.8. Tutorial

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

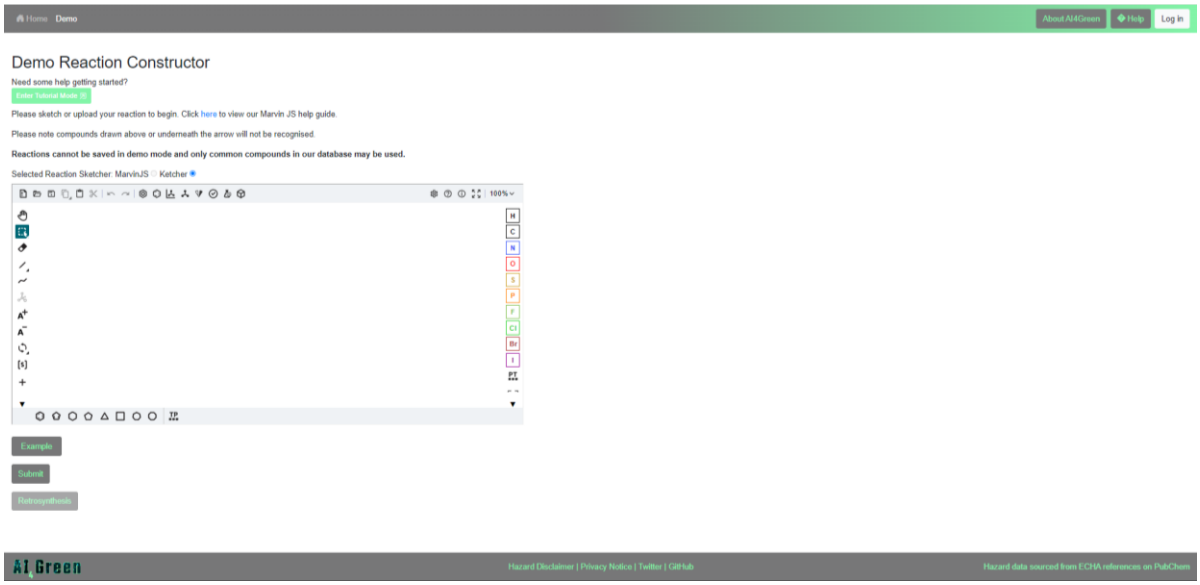


Clicking the “Reaction Builder Tutorial” button initiates the tutorial, which guides you through each of the elements.



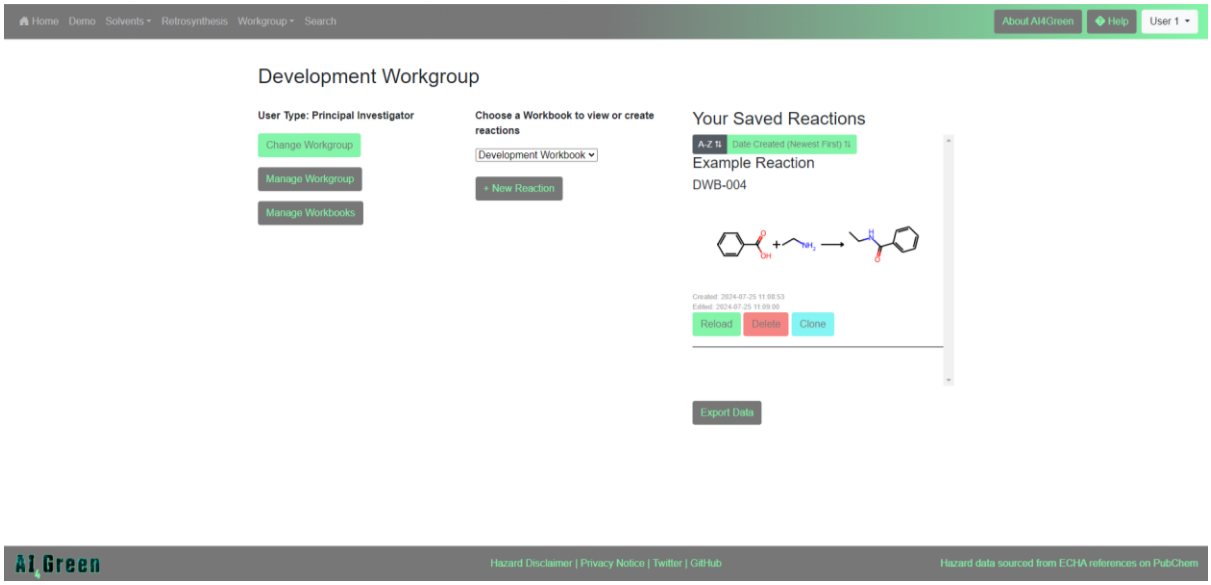
5.9. Demo

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.



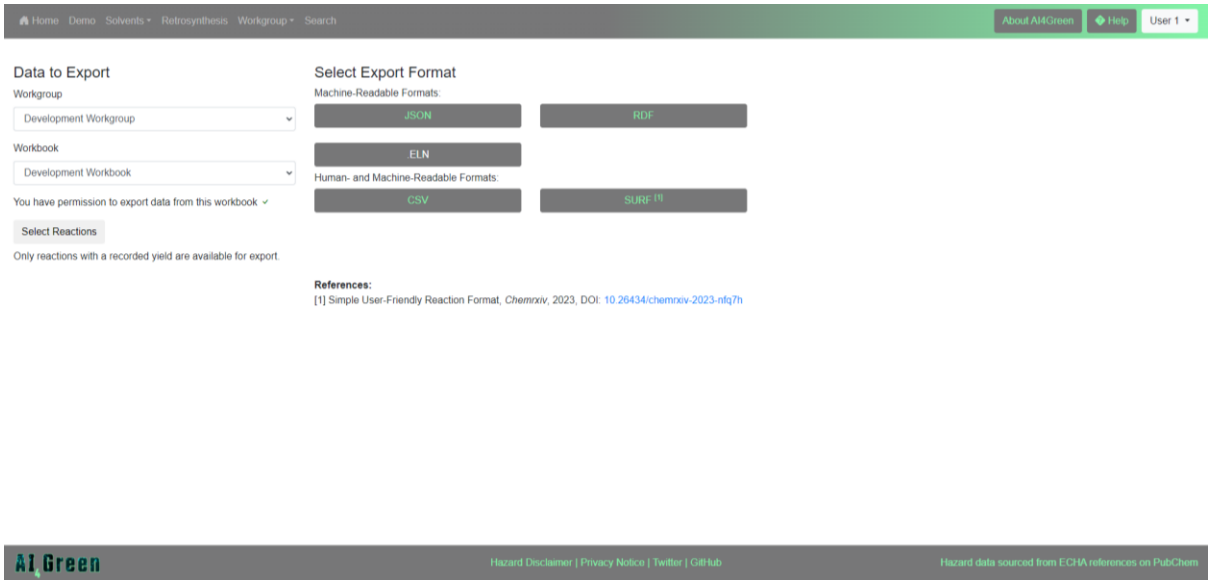
5.10. Exporting Data

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.

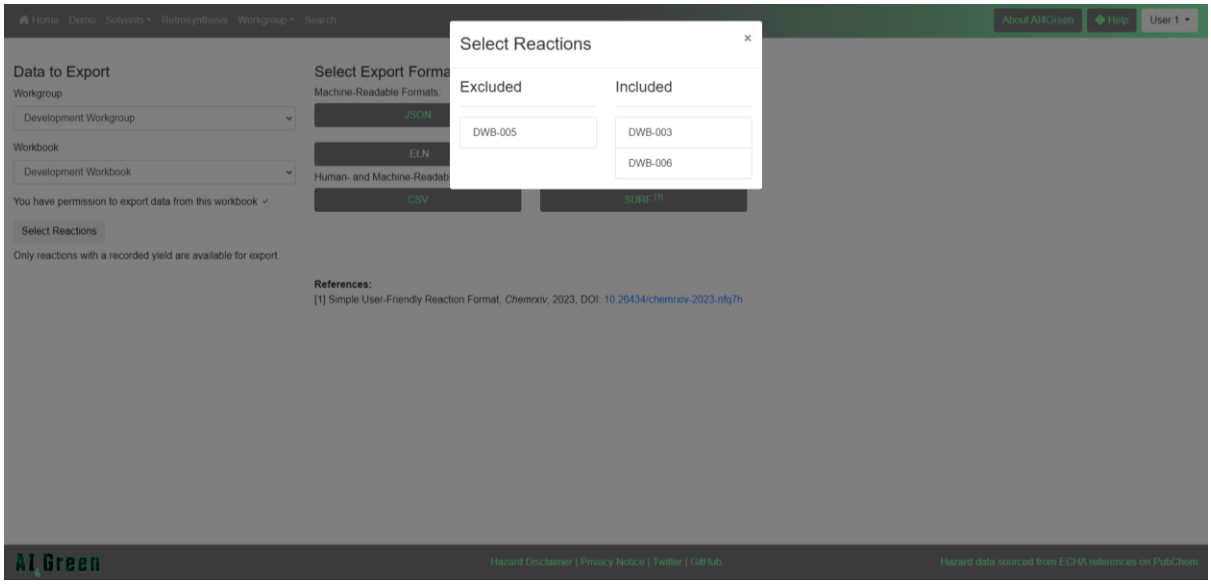


This takes you to the Export Data page, which allows you to export your data in different human and machine-readable formats. All Workbook members have permission to export data from their Workbooks, and Principal Investigators can export from any Workbook in their

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



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.



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

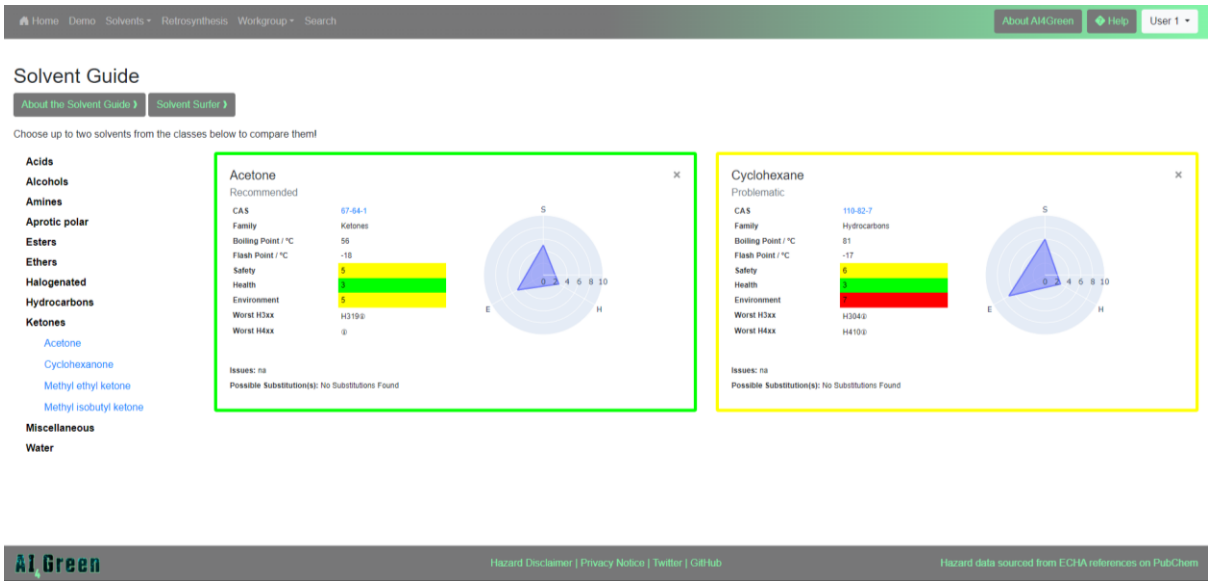
This file stores Reactions as reaction blocks, which are lists of a reaction's atoms and their connectivities.

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.

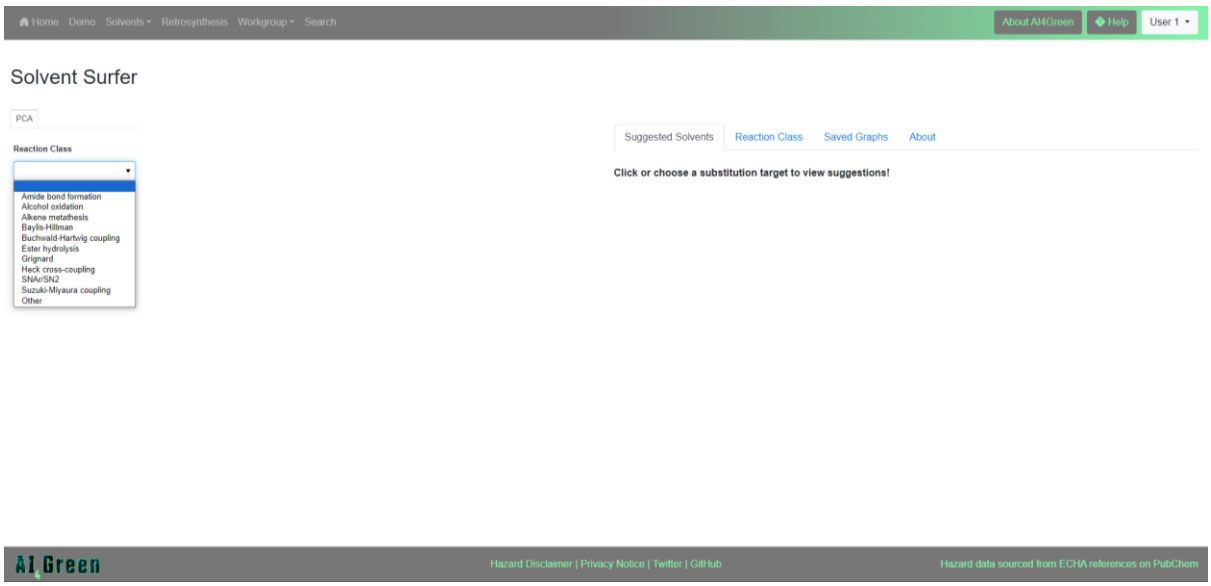


The solvent guide can be accessed from the Navigation bar or by clicking the "Solvent Guide" button when adding solvents to a reaction. The latter option will load the selected solvent in the Solvent Guide for easy comparison.

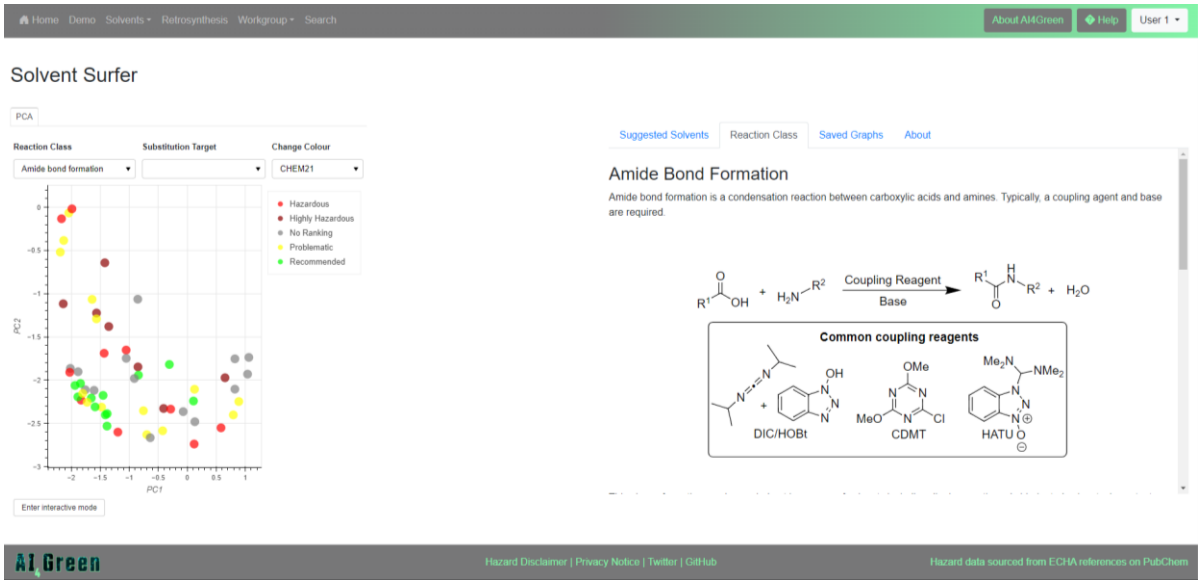
6.2. Solvent Surfer

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.

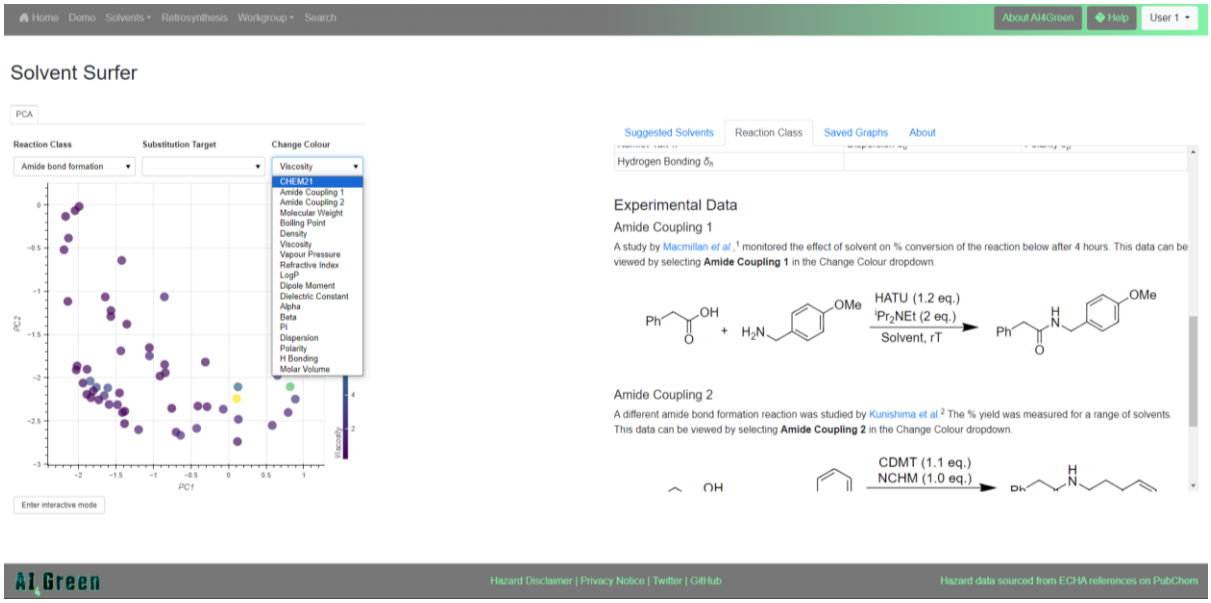
Upon loading the Solvent Surfer page, you are prompted to select a reaction class which generates the corresponding PCA plot.



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.

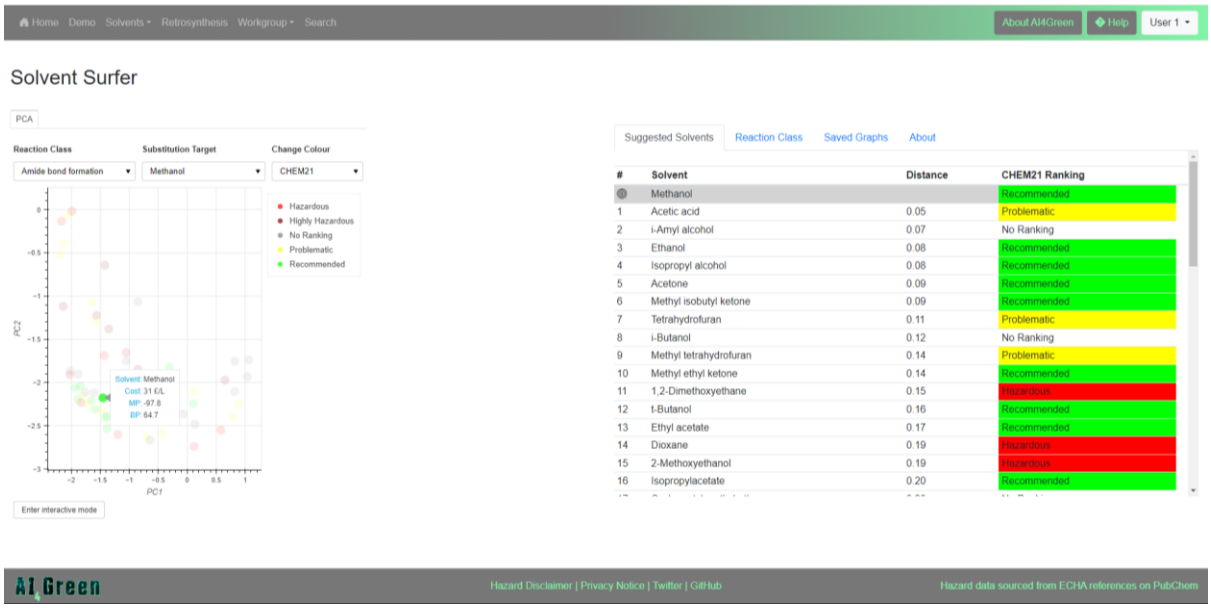


The colours of the data points can also be changed to reflect any of the initial PCA descriptors by selecting a value from the “Change Colour” dropdown. Some experimental data is also included as a colour, and the details of these are provided under the Reaction class tab.



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.

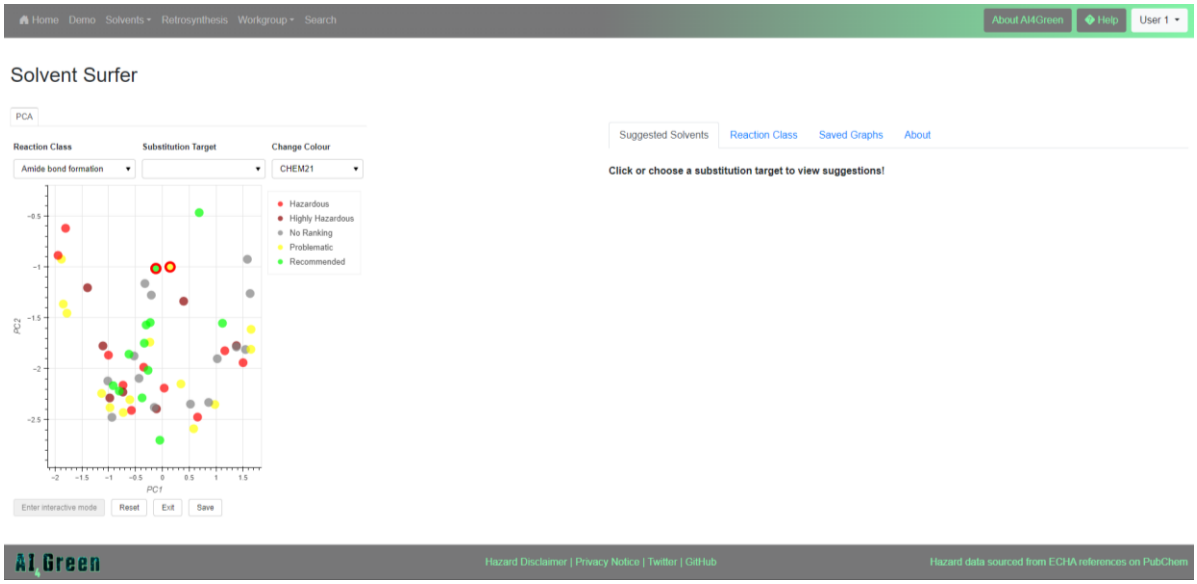


More information about the Solvent Surfer is available under the "About" tab.

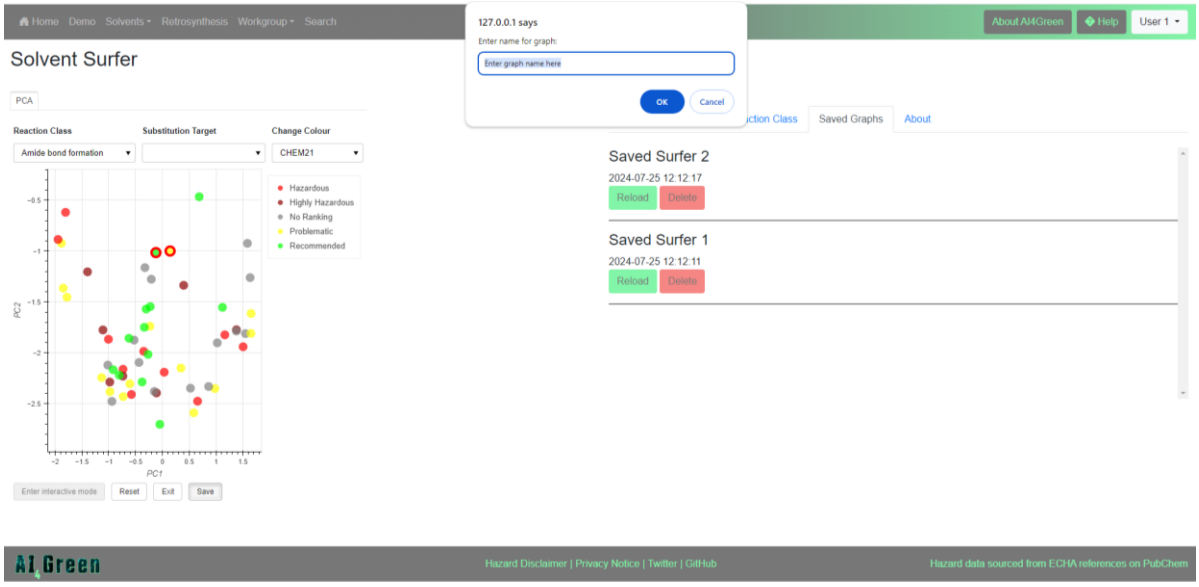
6.2.1. Interactive Mode

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.

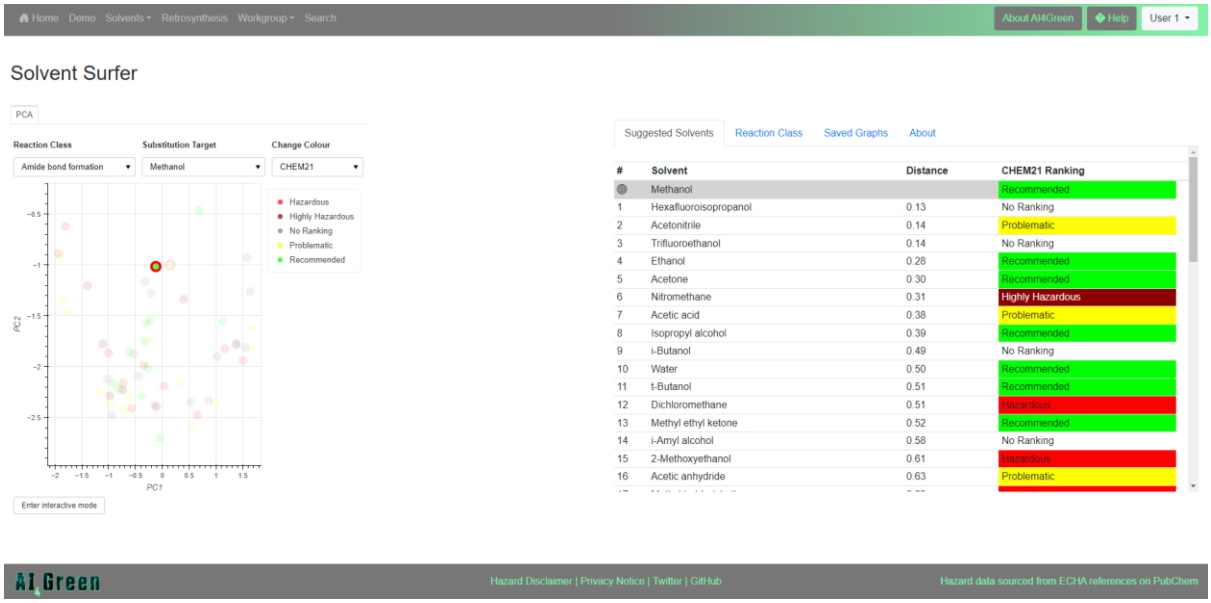


Interactive Surfers can be saved by clicking the “Save” button, where you will be prompted to enter a name for your updated graph. Saved Surfers can be viewed under the “Saved Graphs” tab. These can easily be reloaded or deleted. Note that deleted graphs are archived, so while they are no longer seen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



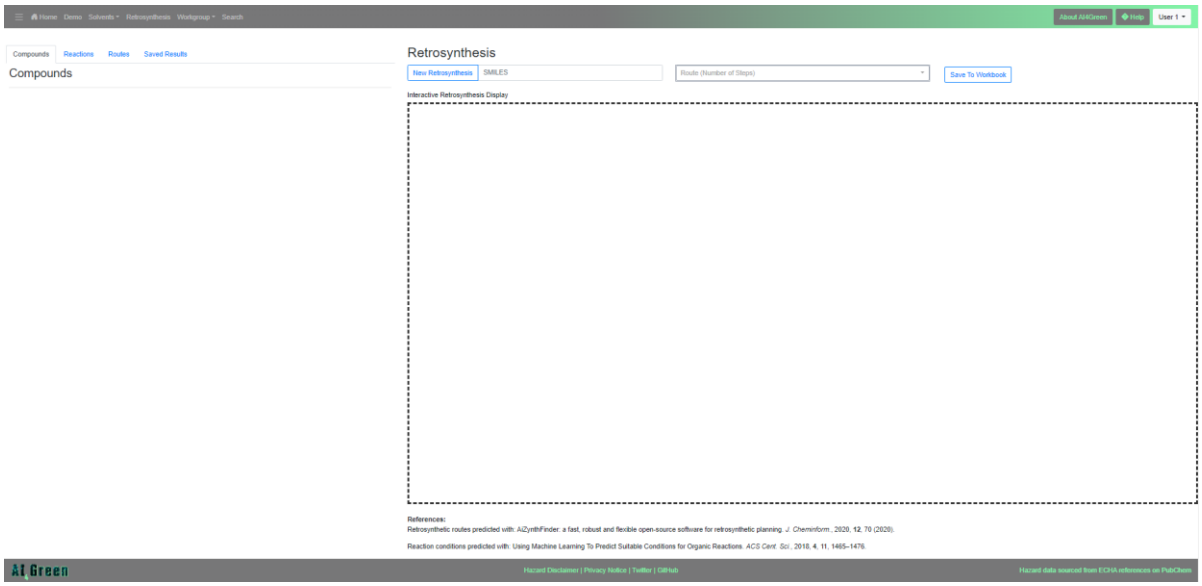
Updated graphs can be reset using the “Reset” button, which reverts the PCA graph back to its original state. This cannot be undone, so please ensure any saved changes are made before clicking this button.

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.



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.

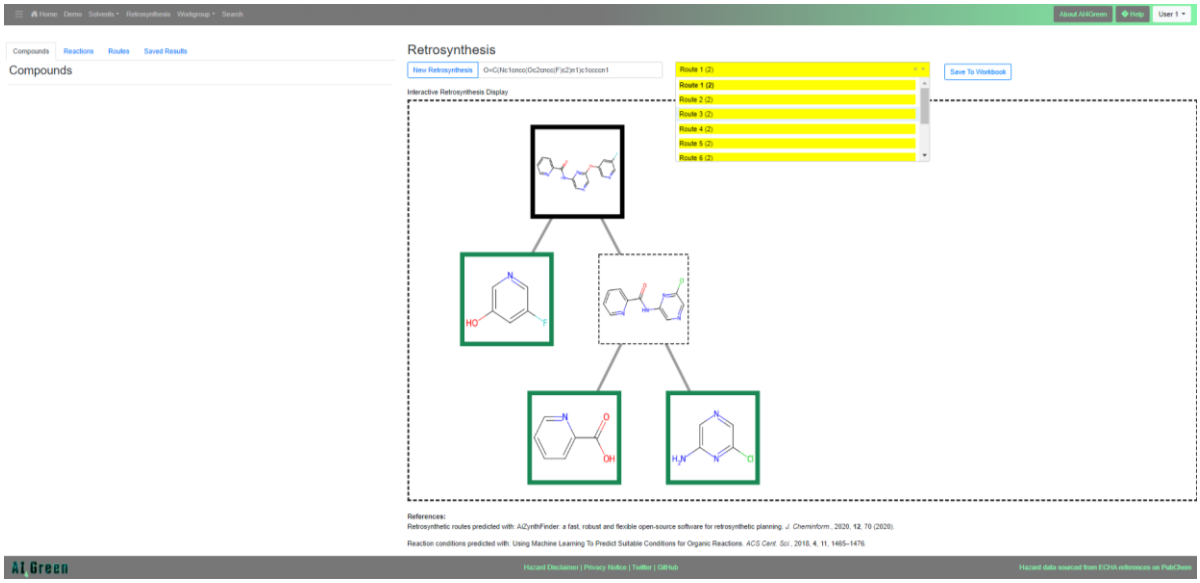


7.1. How it Works

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.

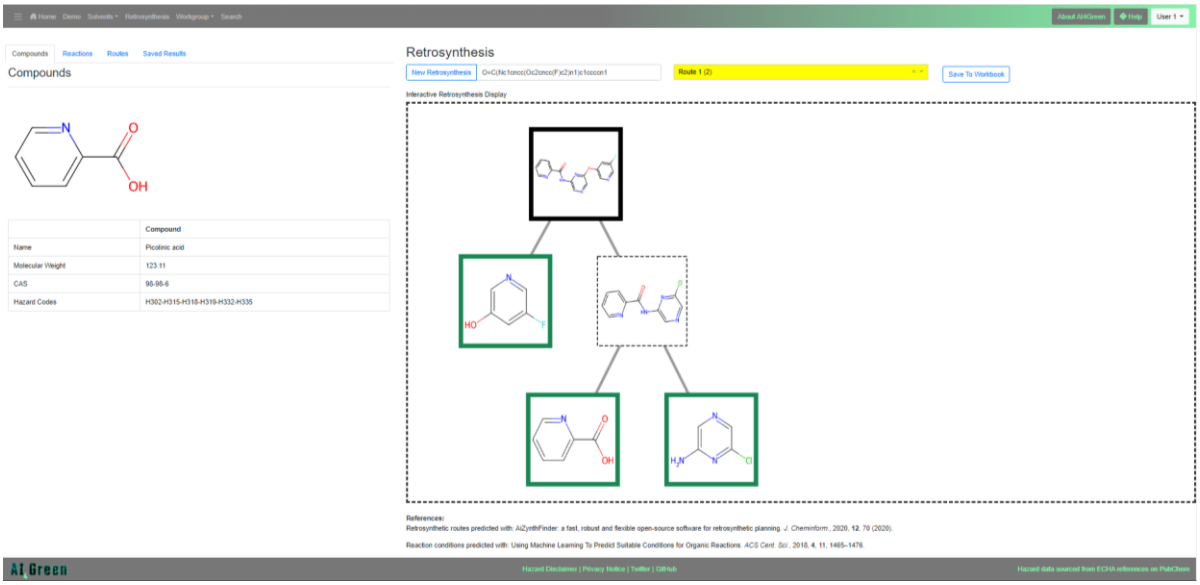
A dropdown with a list of up to ten routes is colour-coded by their sustainability and number of steps in brackets. Different routes can be explored by clicking one of the options from the dropdown.



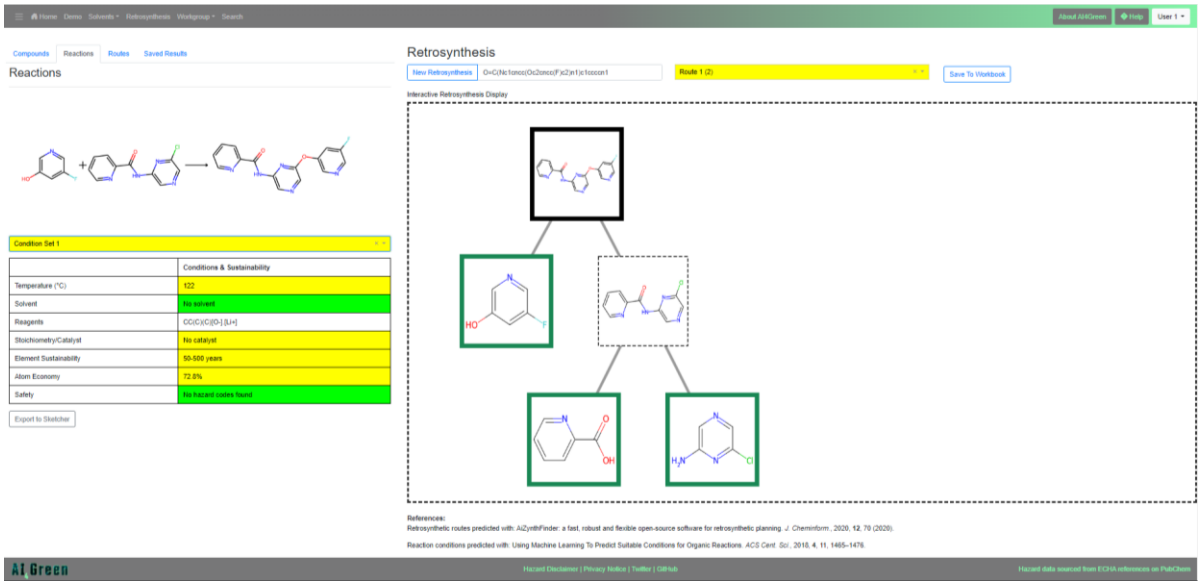
7.2. Analysis

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.

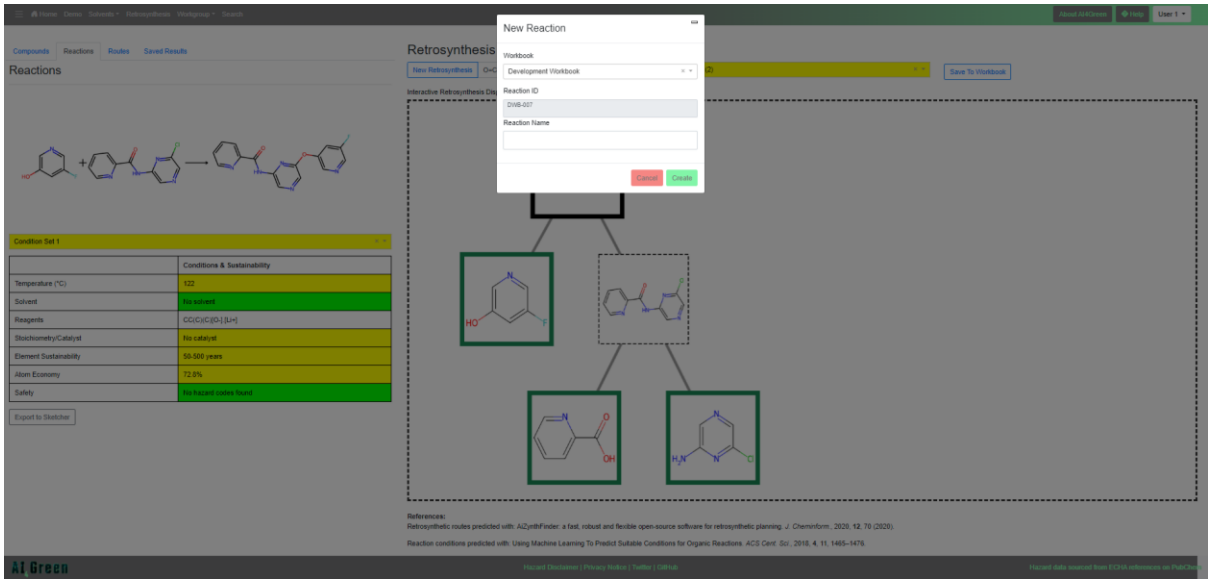
The **compound** tab draws from the AI4Green database to show CAS number, name, hazards, and molecular weight.



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.

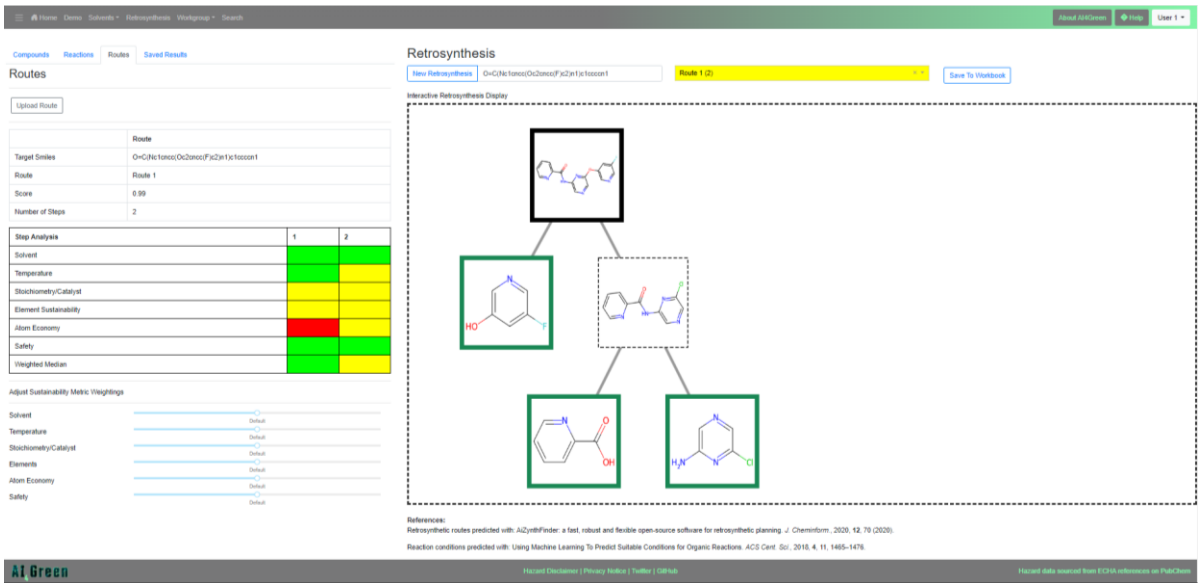


Reactions can be exported to the sketcher from the reaction tab. This allows you to create a new Reaction in your workbook.



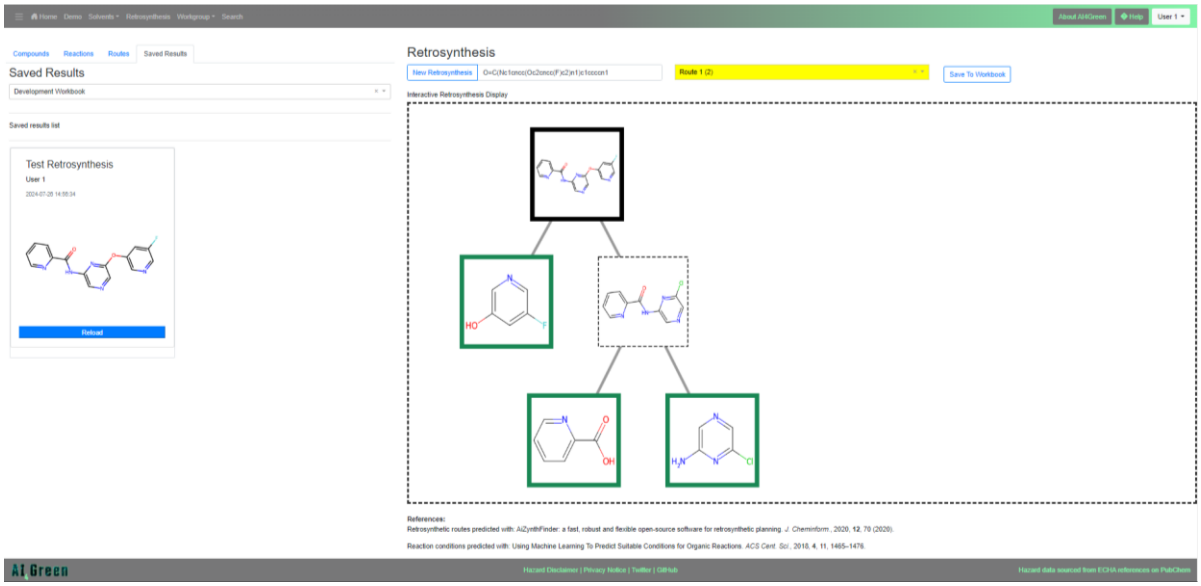
The **route** tab displays an overview of the sustainability of each reaction step for each metric. This is also where the sliders are to adjust the weightings of the metrics which updates the weighted median used to colour reactions and routes.

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



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.



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.