A group of people working in a lab

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AI4Green User Manual

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# Introduction

AI4Green4Students is a pedagogical version of AI4Green (a web application for industrial organic Chemists and researchers). Its primary objective is to encourage learning and application of sustainable chemistry in the undergraduate teaching laboratory. It is integrated with a suite of features that enable the undergraduate organic chemists to plan and document their lab experiments in a collaborative method, allow instructors to oversee and manage projects, as well as monitor students’ progress via consistent review and provision of feedback, and support AI-powered analysis to enable sustainability practices.

The AI4Green4Students web app functions as an electronic lab notebook (ELN) for synthetic organic chemistry and its core component is The Reaction Builder. It has four main sections:

* The learning section,
* The planning section,
* The experiment documentation section,
* The experiment report section.

Future components to be added include:

* Machine Learning-driven Alternative Reaction Pathway Exploration
* AI-powered assessment feature for report evaluation

**Hazard Disclaimer and Privacy Notice**

Note that hazard data was sourced from the European Chemicals Agency ECHA references on PubChem.

**Shared Legal Notices**

The hazard disclaimer and privacy notice applicable to the AI4Green4Students app are those of the parent app, AI4Green. These notices are designed to protect your safety and personal information while using the app. They can be found here: <https://ai4green.app/auth/hazard_disclaimer> and

<https://ai4green.app/auth/privacy_notice>

**Repository Status**

**Independent Repository**: While the AI4Green4Students app is a version of the parent app, it is maintained separately and is not included in the parent app’s repository. This means that any updates or modifications specific to the app are handled independently.

# Getting Started

We have a QuickStart Guide video, accessible from the home page or the Help page. This is intended to help first-time users with the basic functionality of AI4Green4Students.

AI4Green4Students can be accessed at <https://ai4green4students-uat.azurewebsites.net/> from your web browser. We highly recommend using Google Chrome.

To start using the app, a user will first create an account. You will be prompted to provide a username, email address and password. Once registered, a user will have two different views depending on the type of role. An instructor and demonstrator have full access to the app functionalities, while a student user can access only the learning section.

For full access to be granted, a student will have to be added to a project group by their instructor. Once joined, they can then plan, build reactions, document experiment notes, and generate reports.

The home page has two different views for students and instructors. The instructor’s page has features to manage users and registration rules, create a project group and invite students to join (Fig 1)

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**Fig 1** Instructor’s home page.

In contrast, the student’s page has no user management features. Instead, it has a learning section which can be accessed by clicking on “learn more” button. It also has features to enable joining a project group.

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**Fig 2** Student’s home page.

# Projectgroup Structure

A projectgroup is a group of users. There are three different user types with different permissions:

* Instructor
* Demonstrator
* Student

With an account created, the user can create a projectgroup and project timeline, including the planning and experiment deadlines if they are the instructor. They can invite other users including students and demonstrators to join the group. Other users apart from the instructors do not have the right to edit the projectgroup. They can only create reactions and document experiment notes if they are students or comment on notes if they are demonstrators.

The projectgroup page displays different views to different users. The instructor and demonstrators see the list of students, the title of their reactions, the project title and action button to either view or request changes to reactions created. The students page displays the title of reactions, the status (whether completed or not), the name of the project and a feature to view, edit or delete reactions or submit a planned reaction for instructor’s comment.

Within projectgroups, there are projectbooks. These are synonymous to student’s paper lab notebook in which they plan different types of reactions for a given project, document experiment notes and write up report. All members of the projectbook must belong to the projectgroup too.

# Projectgroup and Projectbook Management

Instructors can manage a projectgroup. There are two main features to implement changes in the projectgroup membership or user type within a projectgroup.

* User Management
* Project management
* Registration Rules

The “User Management” page allows direct promotion, demotion, and removal from a projectgroup. Note that removal from a projectgroup also removes the user from any projectbooks of which they are members.

If a change has been requested, they will appear in the “Action” tab. The approver(s) will get a notification that a request has been made with a link to the request page. When a decision has been made, the requester will receive a notification on the outcome of their request.

The “Project management” page enables the instructor to invite students to join a projectgroup, create or edit projectgroups.

Users may join a projectgroup from the relevant buttons on the projectgroup page.

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**Fig 3** User and Project Management Features for creating project groups and inviting students to join.

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**Fig 4** A table showing the list of users in a project group.

# App Sections

The web application has four main sections described below.

## Learning section

This section supports students in learning and understanding green and sustainable chemistry. This section offers a large amount of content focused around green and sustainable chemistry and their application in the industry. It bridges the gap in knowledge, especially for those students who did not choose elective sustainable chemistry module in their year1 and 2 and therefore lacked understanding of the subject. It explains the differences between green and sustainable Chemistry and the metrics for their evaluation. The section integrates links to external websites such as American Chemical Society (ACS), pharmaceutical industries, etc. to broaden and deepen their knowledge.

Furthermore, there is a provision for self-evaluation to gauge the level sustainability knowledge acquired before engagement with creation of sustainable reactions. Once students have explored this section, they can then click on the available projects on the home page and proceed to their project group page. On this page, students can access group activity page and project book.

## Group Activity Section

This section has features that encourage collaboration among students. It provides opportunities for the projectgroup members to brainstorm together, plan and decide what each of them does each week. It also offers support for results analysis and calculations. The number of columns to the right of the tables below is premised upon the number of students in the group. Once the group activity is completed, the student can then proceed to a projectbook to plan experiments.

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**Fig 5** Project Group Activity Page for members in a project group to collaborate.

## The Projectbook

Students use this space to complete all the pre-lab tasks, document experiment notes and write reports. It has three main sections: the planning, Lab note and report sections. Projectbook is a student’s lab notebook but in digital format.

## Planning Section

This section enables students to plan each reaction they will create in the lab. Each plan is saved and can be retrieved for editing before experimenting in the lab. During the planning process, the hazard code is validated for the students. Once all planning is complete, the instructor receives a notification to review. They then assess the plan and input feedback into the comment box shown below. The students then make all the necessary corrections and re-submit to the instructor for approval. Upon approval, the students can then proceed to execute the experiment in the lab.

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**Fig 6** Part of a COSHH Form.

The planning page has four main sub-sections for easy maneuvering: literature review, reaction Scheme, Control of Substances Hazardous to Health (COSHH) form, safety data and experiment procedure.

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**Fig 7** Literature Review section.

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**Fig 8** Experiment Plan Overview Page.

The reaction scheme enables students to construct reactions. The COSHH form collects details of health and safety issues and mitigating procedures for a given reaction. The safety Data is space for additional health and safety issues not recorded on the COSHH form. The Experimental Procedure is a text area for the students to write detailed protocols for the reaction they are creating.

## Lab notebook Section

This section has features that enable students to conduct detailed documentation of experiment notes. The start and end time of a reaction together with duration, conditions and name can be recorded. The purification steps, as well as product characterisation can be recorded. There are also features to export notes and request instructor’s support before report write-up.

The Lab notebook is invisible to students until the completion and submission of the experiment plan. Once approved, the lab notebook becomes activated. It is split into sections which serve as prompts to remind students of the required details to record for accurate reporting.

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**Fig 9** Lab Notebook page Overview showing different subsections.

The metadata allows students to record important information about an experiment which can facilitate the recreation of reactions and publishing.

The reaction scheme enables students to draw the reaction scheme and add quantities of substances used.

The calculate yield and green metrics section is for working out the moles of reactants and products and then calculating the product yield. Students also utilise this section to calculate green metrics for sustainable evaluation of reactions

The TLC Analysis is for discussing the results of TLC analysis as the reaction progresses. There is a button for uploading pictures of the TLC plate to support discussions.

The characterisation of the product is for recording a description of the product including the physical forms, the functional groups, etc. There is a button within this field to upload spectra data such as NMR, IR and MS.

Observation and Inference space is for adding observations noticed as reactions progress and the inference that can be drawn from them.

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**Fig 10** A Cross Section of a Lab Notebook showing Features for yield and Green Metrics Calculations.

## Report Section

In this section, the students create a detailed and structured report of their experiment. It has features that enable viewing and copying both the planning and lab notebook sections. It is split into sections (as shown below) to facilitate easy recollection of key information to include in a formal report.

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**Fig 11** An Overview of Report Section.

# Reaction Builder

To build a reaction, a user must navigate to the projectgroup page from the home page. Then the user must select a new plan and use the “Reaction Scheme” button. Once the reaction is created it can be saved and stored for future reference using the save button and can be reloaded from the projectgroup page.

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**Fig 12** A sketcher pad for drawing compound structure.

The reaction constructor uses the Ketcher chemical drawing package to enable the drawing of a reaction. For more on how to use it click on the question mark/help button which will take you to Ketcher Overview on GitHub.

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With the reaction drawn, it can be processed into a full reaction by clicking the “Generate reaction data” button. It is not currently possible to draw reagents or solvents over/under the arrow. These can be added manually to the reaction table in the next step. The reaction that has been drawn is interpreted as SMILES strings and the relevant molecule information (such as name and density) is pulled from the PubChem database to populate the reaction table. The SMILES string generates the IUPAC name of the molecule using the chemical identity resolver and the molecular weight is automatically calculated and filled in using RDKit.

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The automatically filled reaction table can now be edited. The amounts of each reactant can be adjusted, and other additions made to the reaction — solvent, reagents, catalysts and hazard codes.

The app validates the hazard code using information from the PubChem database. If incorrect codes are entered a comment box pops up at the side with a warning: “Incorrect hazard codes”. The user can then decide whether to check and make corrections or not before submission for assessment by the instructor. The correct hazard code is never provided by the app as this exercise is to enable critical thinking and reasoning.

The limiting reactant can be indicated using a check box and its mass entered. The amounts including that of the products can be calculated from which yield is then calculated. The drop-down button can be used to select the physical states of the substances.

Reagents can be searched for by entering their partial name which will return a list of reagents containing that phrase, their full name to retrieve the exact reagent or their CAS number. If no reagent is returned, it is not in the PubChem database and needs to be added via the sketcher. Depending on the entry in the PubChem database you may need to manually enter the density of any liquids.

Selecting a solvent to add opens a searchable interactive dropdown. 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. Solvents can also be searched for by entering their CAS number.

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Physical forms for each component can be entered via a dropdown menu. The selected option contributes to the hazard rating of a compound.

Once all sections of the reaction table are completed, a user can then complete the COSHH form, the safety data and the experiment procedure of the planning section before submission to an instructor.

# Export Data

Experiment data can be exported from the projectgroup page. There is the option to export the entire projectbook, planning section, lab notebook or report section as a CSV file or For Print/PDF.

# Appendix

## Hazard Disclaimer

Whilst all efforts have been made to provide highly accurate compound data, we cannot accept responsibility for the accuracy or validity of any data provided or any incidents which may occur. The experimental chemist and their supervisor/organisation bear responsibility to be aware of and account for the hazards of all chemicals they are working with and to perform any experiments safely and adhering to the safe working practices set out by their organisation.

All compound data used has been collected from PubChem laboratory chemical safety sheets (LCSS). The hazard data are presented as a global harmonised system of classification and labelling of chemicals (GHS) hazard codes. The hazard data is only collected from the references provided by the European Chemicals Agency (ECHA). More information can be found at: <https://pubchemdocs.ncbi.nlm.nih.gov/lcss>

## AI4Green Privacy Policy

**Our contact details**

Address: School of Chemistry, University of Nottingham, Nottingham, NG7 2RD

Email: [admin@ai4green.app](mailto:admin@ai4green.app)

**The type of personal information we collect**

We currently collect and process the following information:

Personal identifiers and email (for example, name, institution, website user information, error logs and contact details)

**How we get the personal information and why we have it**

The personal information we process is provided to us directly by you. We use the information that you have given us in order to manage your account, personalise your use of the website, and manage your workbook, workgroup, and institution affiliation.

We won’t share this information with anyone else.

Under the UK General Data Protection Regulation (UK GDPR), the lawful bases we rely on for processing this information are:

**(a) Your consent. You are able to remove your consent at any time. You can do this by contacting**[**admin@ai4green.app**](mailto:admin@ai4green.app)**.**

**(b) We have a legitimate interest.**

**How we store your personal information**

Your information is securely stored.

We keep all personal information whilst your account is active. We will then dispose of your information when a request is made to remove your account or after 2 years of inactivity. Upon removal of your personal data, your reaction data will be retained and anonymised.

**Your data protection rights**

Under data protection law, you have rights including:

**Your right of access** - You have the right to ask us for copies of your personal information. Upon creating your account, you gain access to view your personal information at any time through AI4Green Account Management.

**Your right to rectification** - You have the right to ask us to rectify personal information you think is inaccurate. You also have the right to ask us to complete information you think is incomplete. Upon creating your account, you gain access to edit your personal information at any time through AI4Green Account Management.

**Your right to erasure** - You have the right to ask us to erase your personal information in certain circumstances. Upon creating your account, you gain access to request your account deletion at any time through AI4Green Account Management.

**Your right to restriction of processing** - You have the right to ask us to restrict the processing of your personal information in certain circumstances.

**Your right to object to processing** - You have the the right to object to the processing of your personal information in certain circumstances.

**Your right to data portability** - You have the right to ask that we transfer the personal information you gave us to another organisation, or to you, in certain circumstances.

You are not required to pay any charge for exercising your rights. If you make a request, we have one month to respond to you.

Please contact us at [admin@ai4green4students.app](mailto:admin@ai4green4students.app) if you wish to make a request.

We may change this Privacy Policy from time to time, so it is advisable to review it frequently. Changes to this Privacy Policy will be announced on the AI4Green Website, all amended terms shall automatically be effective [7] days after announcement.

**Cookies**

This website uses first-party cookies to optimise the user experience by tracking sessions and remembering user information and preferences.

**How to complain**

If you have any concerns about our use of your personal information, you can make a complaint to us at [admin@ai4green.app](mailto:admin@ai4green.app).

You can also complain to the ICO if you are unhappy with how we have used your data.

The ICO’s address: Information Commissioner’s Office, Wycliffe House, Water Lane, Wilmslow, Cheshire, SK9 5AF

Helpline number: 0303 123 1113

ICO website: [https://www.ico.org.uk](https://www.ico.org.uk/)