AI4Green User Manual

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Introduction

AI4Green is a webapp to enable synthetic organic chemists to record their work in a collaborative method, allow principal investigators and supervisors oversight of work performed, and enable synthetic pathway analysis to enable the exploration of alternative, “greener” reactions.

The AI4G webapp functions as an electronic lab notebook (ELN) for synthetic organic chemistry and its core component is The Reaction Constructor.

Future components to be added include:

1. The Solvent Selector (Solvent information flashcards are currently available)
2. The LCA Green Metrics Analysis
3. Machine Learning driven Alternative Reaction Pathway Exploration

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

Getting Started

We also have a Quickstart Guide, accessible from the home page or the Help page. This is intended to help first time users with the basic functionality of AI4Green.

AI4Green can be accessed at https://ai4green.app/ from your web browser. We highly recommend using Google Chrome.

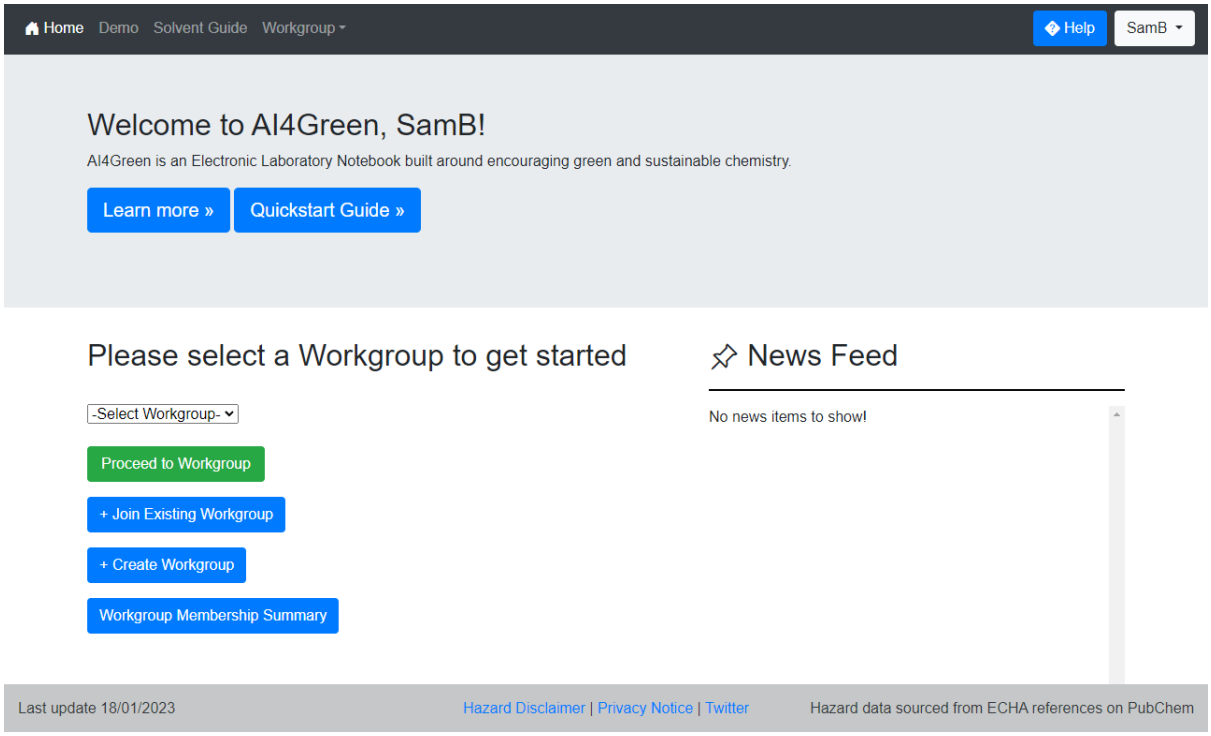
The first step to using the AI4Green webapp is creating an account. You will be prompted to provide a username, your full name, email address, and password.

Once registered, a user has access to the full functionality of AI4Green.

The home page displays: options for selecting and proceeding to a workgroup page; joining a workgroup; checking workgroup membership; and creating a workgroup.

The top navigation bar has links to the home page; demo reaction construction (all the features of the reaction constructor but reactions cannot be saved and novel compounds cannot be added); solvent guide; a dropdown of workgroups the user is a member of; help page; and user dropdown (notifications, change hazard colours on the accessibility page, the option to login/logout, and change email/password).

There is also a news feed displaying messages from admins.



Workgroup Structure

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

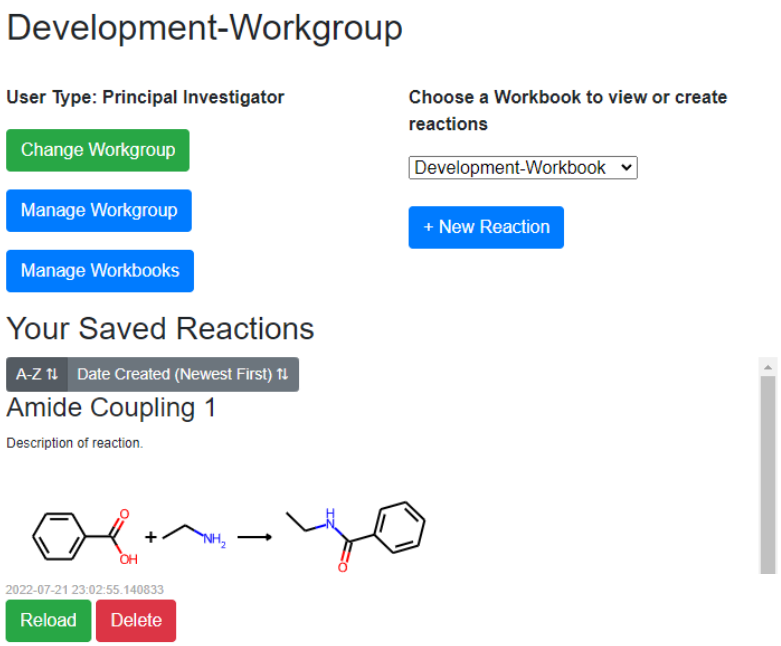
- Principal Investigator
- Senior Researcher
- Standard member

With an account created the user will be able to join existing workgroups or create their own if they are the principal investigator/leader of a workgroup. In the first instance of joining a workgroup the user is set as a "standard user". This means that they can use the webapp to construct and save reactions, but they cannot create new workbooks within that workgroup or add/remove other users. When a user creates a workgroup, they will become the principal investigator of that workgroup.

The workgroup page shows the user's user type, a dropdown with the workbooks they belong to and a scrollable list of the saved reactions in that workbook.

Reactions can be sorted A-Z or by date created (newest first). There is also the option to delete a reaction. Note that deleted reaction may not be able to be recovered.

Depending on the user type, additional options may be visible. Senior researchers and principal investigators can access Manage Workbooks and only principal investigators can access Manage Workgroups.



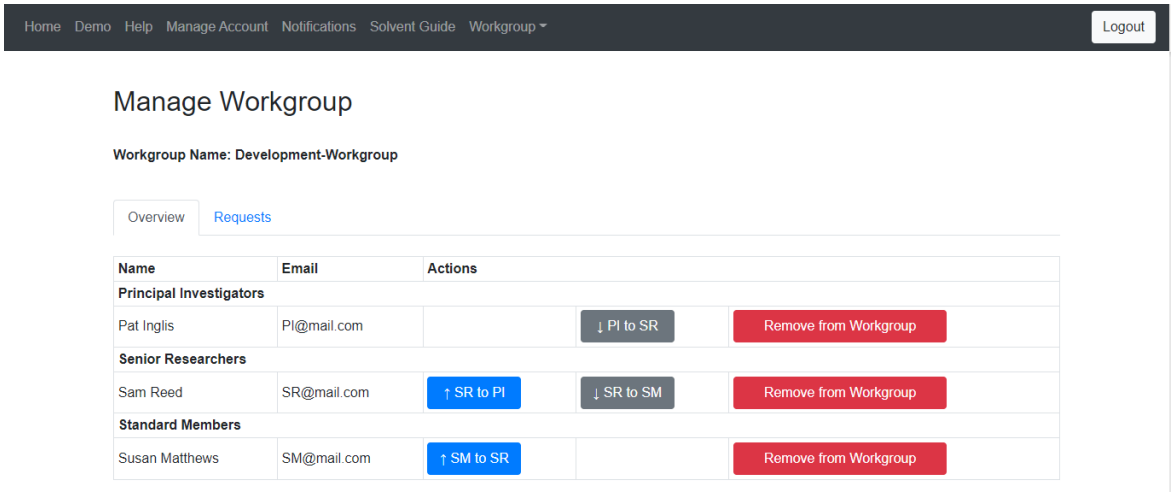
Within workgroups, there are workbooks. These are collections of reactions intended to be from a single project. There can be multiple workbooks within a workgroup. All members of the workbook must belong to the workgroup too.

Once a user is a member of a workgroup and workbook they can make, save, and reload reactions and add their own novel compounds.

Workgroup and Workbook Management

Principal investigators can manage a workgroup and both principal investigators and senior researchers can manage workbooks. There are two ways to change workgroup/workbook membership or user type within a workgroup.

- By the principal investigator or senior researcher in the “Manage Workgroup” or “Manage Workbook” pages
- By the researcher requesting a change in status



The “Manage Workgroup” page allows direct promotion, demotion, and removal from a workgroup. Note that removal from a workgroup also removes the user from any workbooks of which they are members.

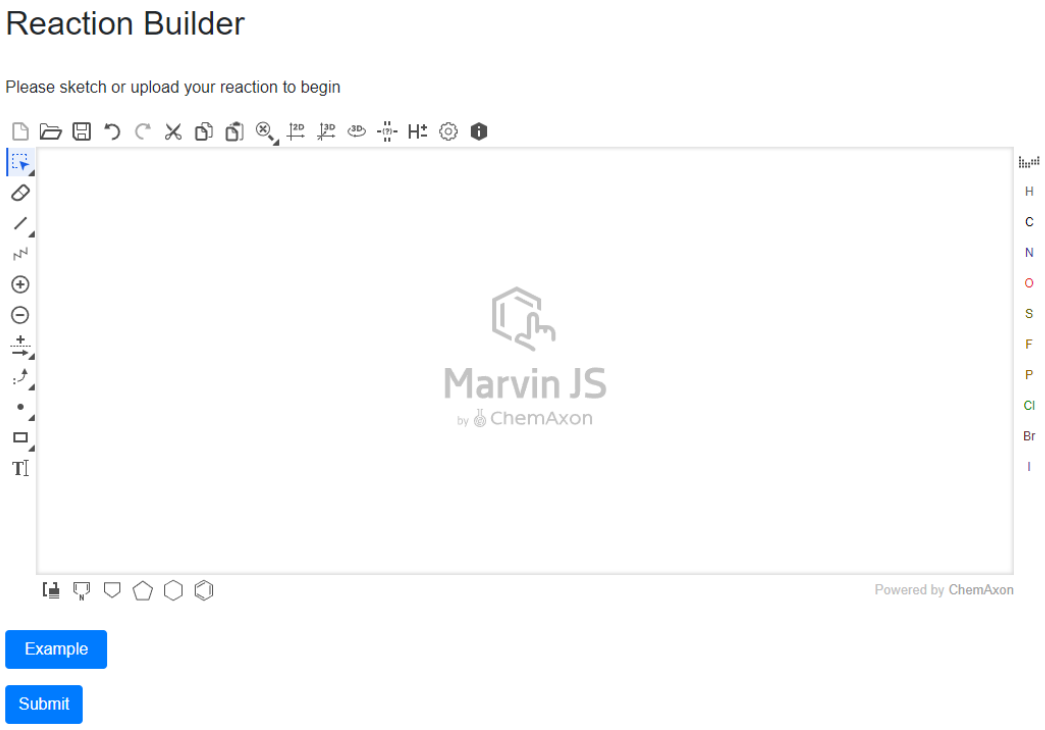
If a change has been requested, they will appear in the “Requests” tab. The approver(s) will get a notification that a request has been made with a link to the request page. When a decision has been made, the requester will receive a notification on the outcome of their request.

This is the same for “Manage Workbook” except users are either “Workbook Members” or “Other members in Workgroup”.

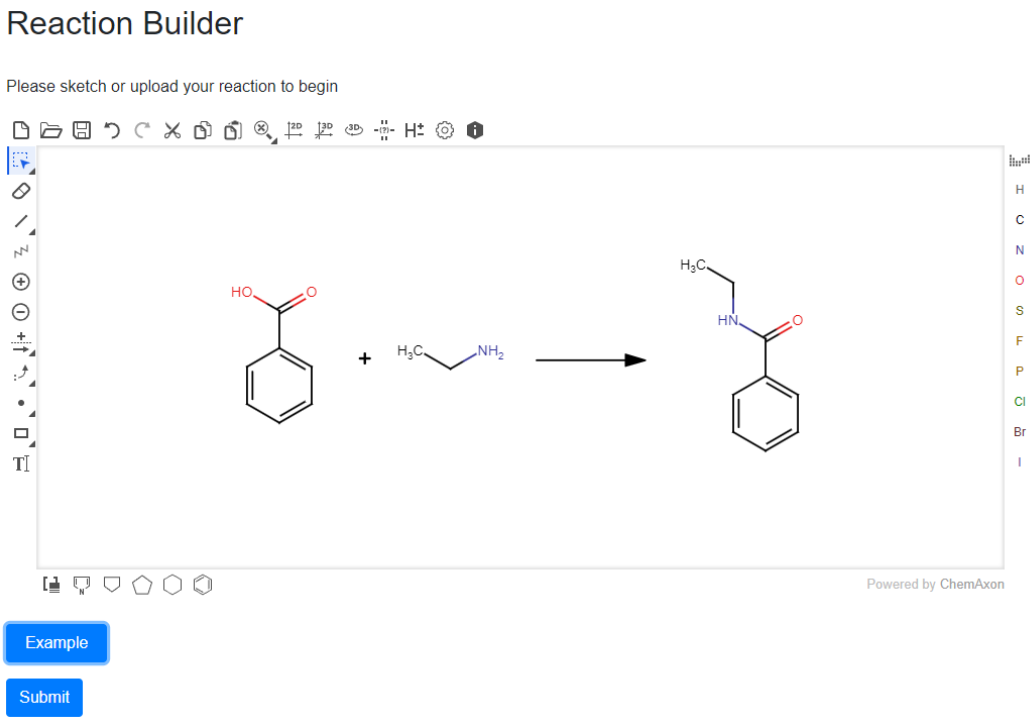
Users may join a workgroup or workbook from the relevant buttons on the home page or workgroup page respectively.

Reaction Constructor

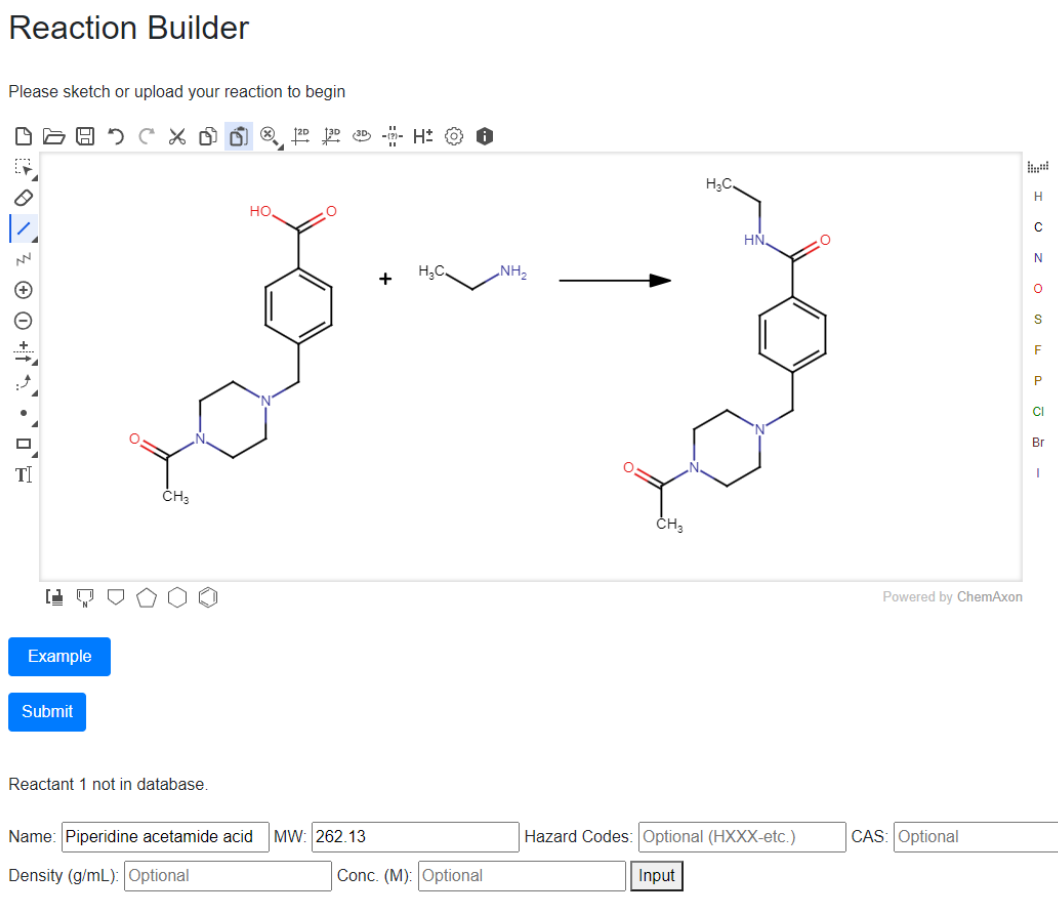
To build a reaction, a user must navigate to the workgroup page. This can be done from the home page or from the “workgroup” dropdown in the navigation bar. Then a user must select the workbook and use the “New Reaction” button. A unique name must be specified for the reaction. Reactions are automatically saved and can be reloaded at any time from the Workgroup page.



The reaction constructor uses the Marvin.js chemical drawing package to enable the drawing of a reaction. For more on how to use Marvin.js refer to our Marvin JS guide on the Help page.



With the reaction drawn it can be processed into a full reaction by clicking the “Submit” 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 is pulled from the PubChem database — or in the case of novel compounds that are proprietary they are drawn from the compounds that are stored in the workbook list of novel compounds. In the event the novel compound is in neither database, you will be prompted to provide as much information as possible regarding this compound. The SMILES string will be used to try and generate the IUPAC name of the molecule using the chemical identity resolver, but this is not always possible; in which case the user must give the molecule a name. The molecular weight will be automatically calculated and filled in using RDKit. Known hazard codes for novel compounds should be entered using a dash as a delimiter, e.g., ‘H301-H331-H302’.



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, and catalysts.

The mass of the limiting reactant can be entered, and the equivalents of the other reactants/reagents are entered and from this the mass/amount/volumes are calculated. The limiting reactant always has an Equiv. of 1, and all other equivalents should be relative to this.

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. 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. Solvents can also be searched for by entering their CAS number.

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

If there is more than one reactant, and more than one product, the radio buttons can be clicked to change which product and which reactant are primary. This is important for determination of yield and the final green metrics of the reaction.

There is space to provide further information that is not captured by the reaction table fields.

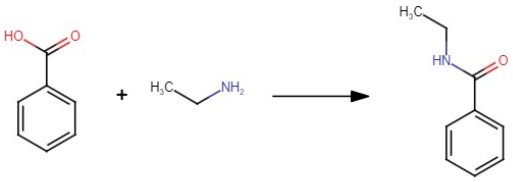
Amide Coupling

Please describe your reaction

Please fill in the highlighted boxes to proceed

№	Reactants	Limiting Reagent?	Mol.Wt	Density (g/mL)	Conc. (M)	Equiv.	Amount mmol	Volume mL	Mass mg	Physical Form	Hazards
1	Benzoic Acid	◉	122.12	-	-	1	-	-	-	-select-	H315-H318-H372
2	Ethylamine	○	45.08	-	-	-	-	-	-	-select-	H220-H319-H335
	Catalysts/reagents Add new reagent to database										Add Reagent
	Solvents Add new solvent to database							mL			Add Solvent
	Product	**Desired Product?**					mmol		mg		
3	N-Ethylbenzamide	◉	149.19				-		-	-select-	H302

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”.



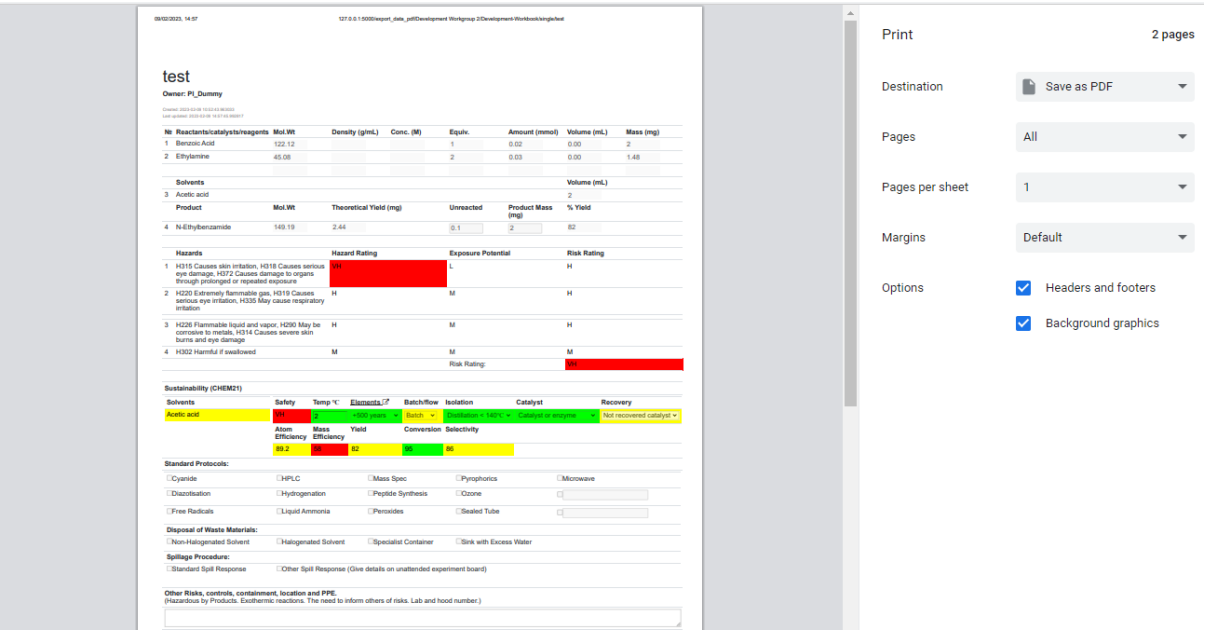
№	Reactants/catalysts/reagents	Mol.Wt	Density (g/mL)	Conc. (M)	Equiv.	Amount (mmol)	Volume (µL)	Mass (mg
1	Benzoic acid	122.12			1	0.82	0.00	100
2	Ethylamine	45.08	0.7		3	2.46	157	111
3	Diisopropylethylamine	129.24	0.742		1.4	1.15	200	148
4	O-(7-Azabenzotriazol-1-yl)-N,N,N',N'-tetramethyluronium hexafluorophosphate	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

In the summary table there is safety information to fill in, information used to determine the sustainability of the reaction using the CHEM21 green metrics, and product mass data for calculating the yield.

Some of these can only be completed after the reaction has been finished. Therefore, a reaction can be saved, and then reloaded and fully filled out when the reaction has been completed. Note that the unreacted and product mass must be entered to mark a reaction as complete. A reloaded reaction can be updated by pressing the update button; this will save any changes to the summary or reaction table.

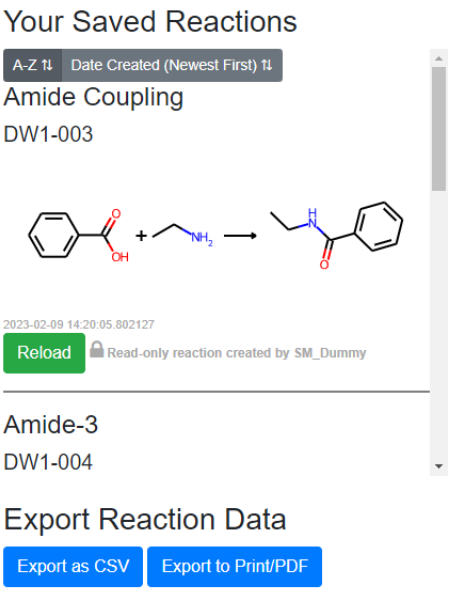
The print summary button will allow you to print the summary table. This contains the reaction scheme & table, hazard matrix, sustainability metrics, additional hazard data, and space for the chemist's and their supervisor's signature. This printout can be taken into the lab and placed near the reaction to act as a reference for the COSHH + H&S data for the reaction.



Colours for solvents and other metrics can be changed from the accessibility page on the user dropdown.

Export Data

Data for a Workbook can be exported from the Workgroup page, below the list of saved reactions on the right side. There is the option to export as either a CSV file or For Print/PDF.



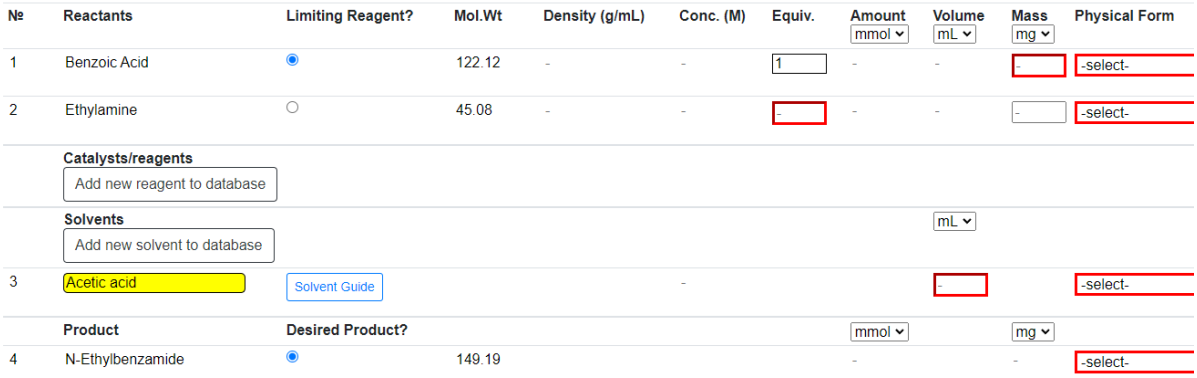
The CSV file contains all the information from the reaction table and summary table and all sustainability elements.

The PDF contains the name, description, time of creation and update, and summary table only.

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

Solvent Guide

The solvent guide can be accessed from the top navigation bar or while building a reaction. The latter option will preload the solvent selected into the solvent guide.



Information about the solvent guide can be found by pressing the “About the Solvent Guide” button.

Further Help

Visit our help page 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.