AI4Green User Manual

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AI4Green User Manual – 03/2024 – Version 1.5

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 AI4Green webapp functions as an electronic lab notebook (ELN) for synthetic organic chemistry and its core component is The Reaction Constructor.

We are excited to announce a beta edition of the solvent surfer has been released. Additional development to increase the number of solvents is in progress.

Future components to be added include:

1. The LCA Green Metrics Analysis
2. Route planning tool with retrosynthetic analysis, condition prediction with an integrated sustainability assessment.
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.

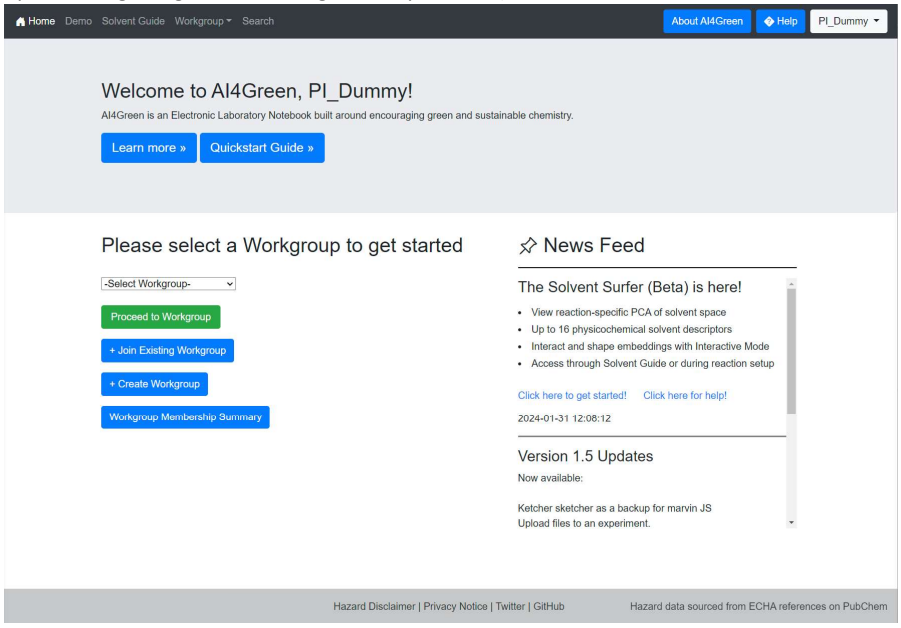
AI4Green can be accessed at https://ai4green.app/ from your web browser. We highly recommend using Google Chrome.

Registering as a New User
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
After logging in, the home landing page for all users displays options for selecting, joining, and creating a workgroup. There is also a news feed displaying messages from admins.

The Navigation Bar
The top navigation bar has links to the home page, demo reaction construction, solvent guide, a dropdown of workgroups the user is a member of, the search function, help page, and user dropdown (notifications, change hazard colours on the accessibility page, the option to login/logout, and change email/password).



Workgroup Structure

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

- Principal Investigator
- Senior Researcher
- Standard Member

After creating an account, the user will be able to join existing workgroups or create their own if they are the principal investigator/leader of a workgroup.

Principal Investigator
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 highly recommend adding at least one additional trusted user as a principal investigator. This ensures efficient management of administrative tasks for the workgroup, particularly in situations where the primary investigator is unavailable.

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.

Standard Member
In the first instance of joining a workgroup, the user is set as a Standard Member. This means that they can construct and save reactions, but they cannot create new workbooks or add/remove other users.

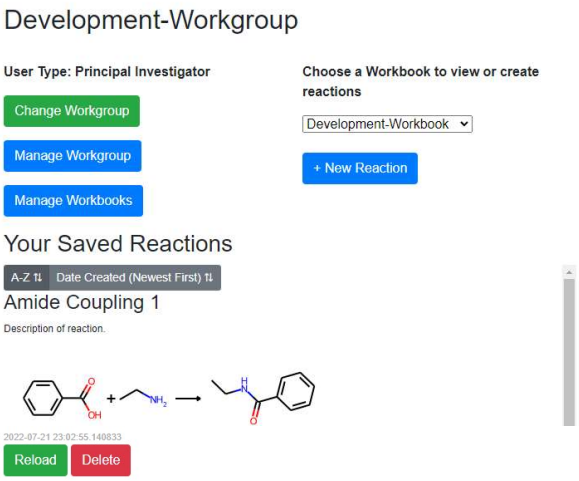
Standard Members can submit a request to the Principal Investigator to be promoted to Senior Researcher.

Note: all users can create and save reactions.

The Workgroup Page
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 alphabetically or by date created. 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.



Workbooks
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.

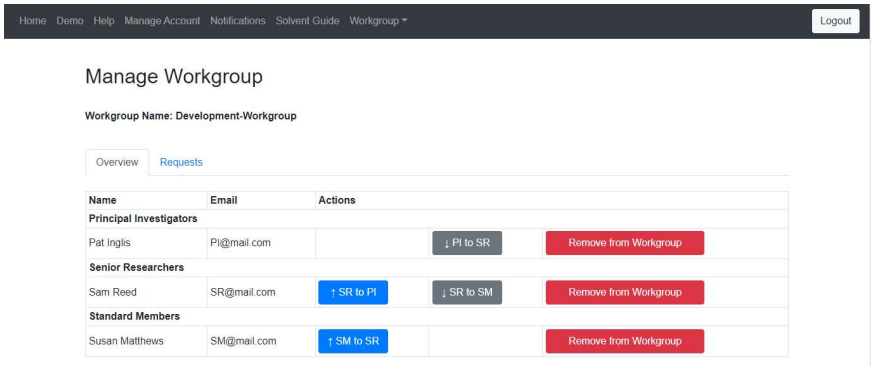
Once a user is a member of a workgroup and workbook they can make, save, and reload reactions and add their own novel compounds.

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:

- The principal investigator or senior researcher can do this in the “Manage Workgroup” or “Manage Workbook” pages.
- The researcher can request a change in status/access.



The Manage Workbook/Workgroup pages
The “Manage Workgroup” page allows direct promotion, demotion, and removal of users from a workgroup.
From the “Manage Workbook” page, you can remove Workbook users, or grant Workbook access to other members of the Workgroup.

Note that removal from a Workgroup also removes the user from any Workbooks of which they are members.

Requesting changes
To request access to a Workgroup, users can select ‘Join Existing Workgroup’ from the Home Page. For access to a Workbook, the relevant button will be found on the Workgroup page.
Accepting changes
Principal Investigators and Senior Researchers will be notified when a user makes a request. If a change has been requested, this will appear in the “Requests” tab. The approver(s) will see a link to the request page on the notification.

When a decision has been made, the requester will receive a notification on the outcome of their request

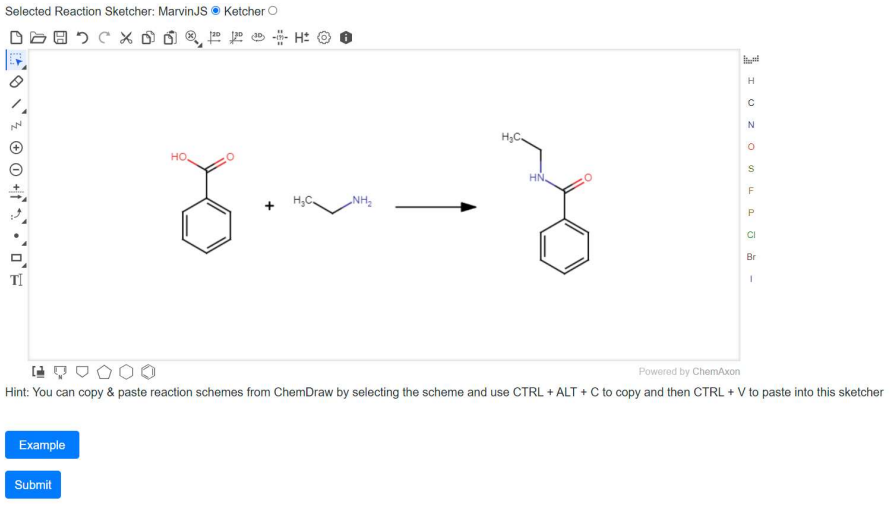
Reaction Constructor

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.

Using the Reaction Sketcher

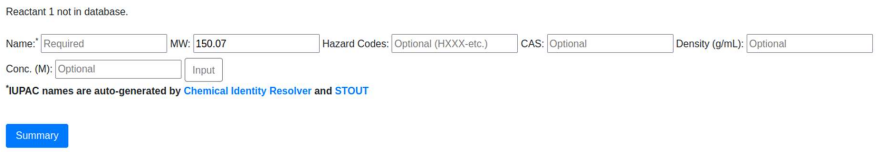
There is a choice of MarvinJS or Ketcher to draw reactions. Use the tutorial button for help getting starting drawing reactions. For more detailed guidance, please refer to the MarvinJS User Manual.



Compound Database

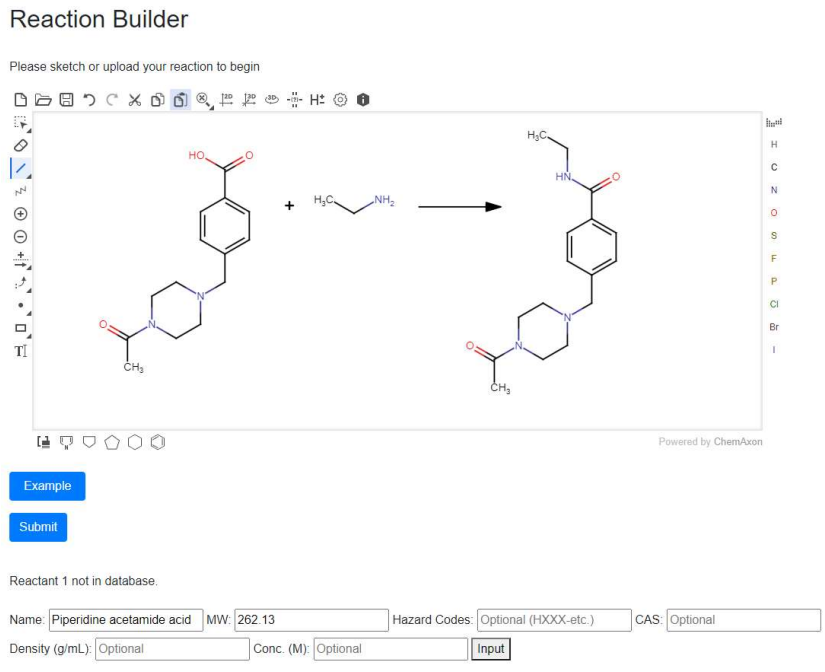
Once a user clicks 'Submit', the reaction drawn in the Reaction Sketcher is interpreted as SMILES strings, and the relevant molecule information (name, hazards etc.) is pulled from the PubChem database.

If a compound is not present in the PubChem database, you can add it to your workbook's Novel Compound database, where it can be accessed again. 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 which 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'.



Reaction Table

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.

Any further information that is not captured by the reaction table fields can be written in the description box above the table.

Mass, Amount, Volume
The mass of the limiting reactant can be entered, along with the equivalents of the other reactants/reagents, 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.

Primary Reactant/Product
If there is more than one reactant, and more than one product, the circular 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.

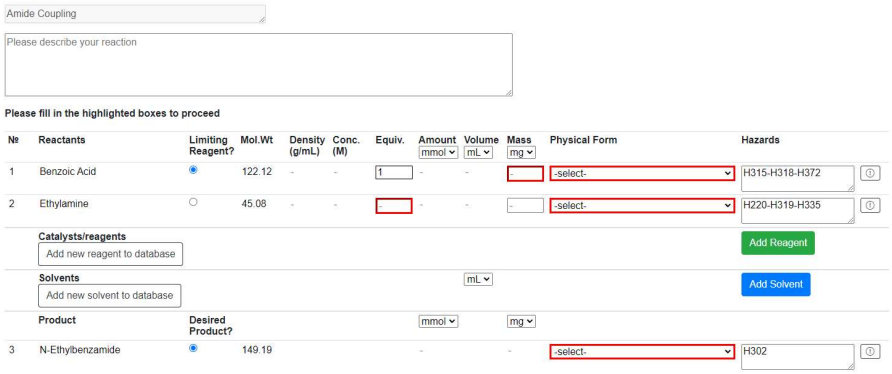
Reagents
Reagents can be searched for by entering their partial name which will return a list of reagents containing that phrase, their full name to retrieve the exact reagent or their CAS number. If no reagent is returned, it is not in the PubChem database and needs to be added via the sketcher. Depending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

Solvents
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.

Commented [JD1]: Colour change opts

Physical Form
Physical forms for each component can be entered via a dropdown menu. The selected option contributes to the risk rating of a compound, which can be viewed after pressing ‘Summary’.


Amide Coupling

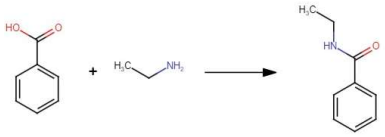
Please describe your reaction

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”.

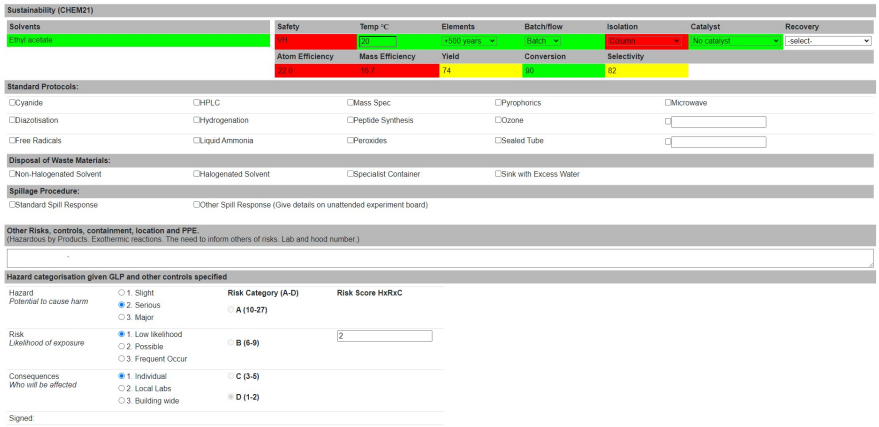
Summary Table



№	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

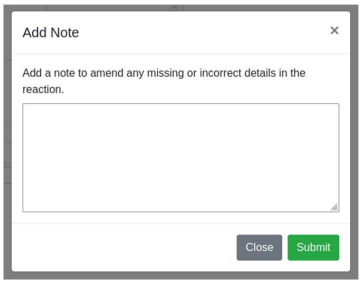
In the summary table there is safety information to fill in, information used to determine the sustainability of the reaction (using the CHEM21 green metrics), and product mass data for calculating the yield.



Completing a Reaction

Some fields in the Summary Table can only be completed after the reaction has been finished. Therefore, a reaction can be 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.

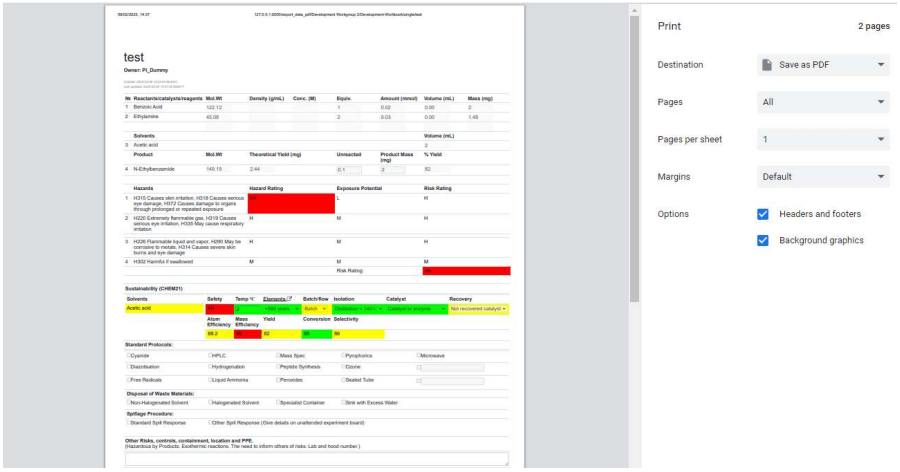
When a reaction is complete and all fields have been filled out, it should be locked to prevent further changes. Note that a reaction cannot be unlocked, but notes can still be added.



Printing the Summary 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.

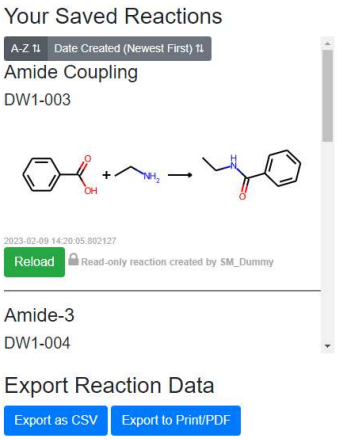
This printout can be taken into the lab and placed near the reaction to act as a reference for the COSHH + H&S data for the reaction.



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.



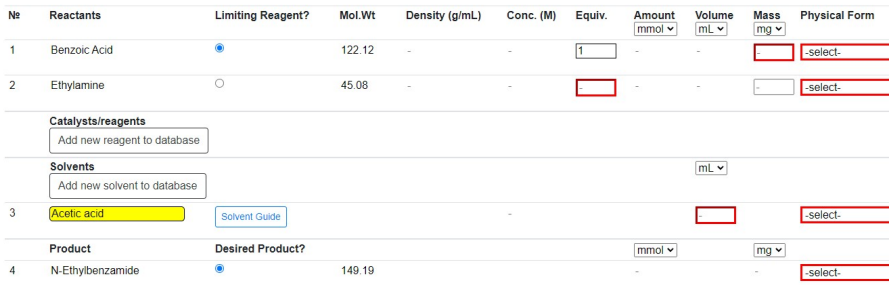
The CSV file contains all the information from the reaction table and summary table, and all sustainability elements.

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.

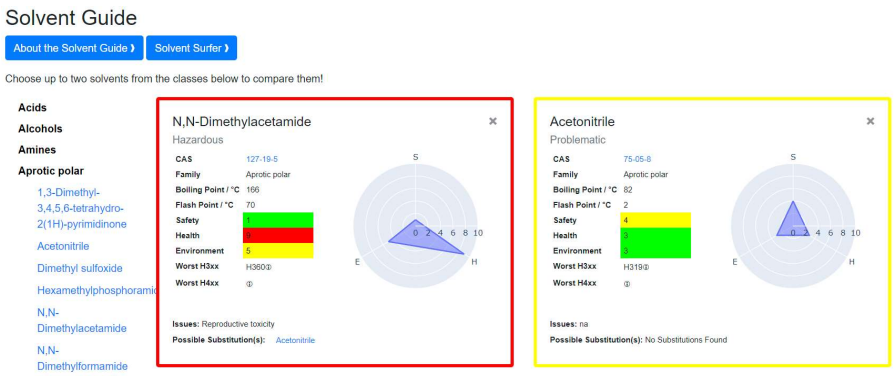
Solvent Guide

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.



In the solvent guide the user can select solvents from the list on the left side of the screen which are grouped by solvent class.

These include some information about the compound including physical properties related to safety, safety, health, and environment rankings from CHEM21, and recommended substitutions.

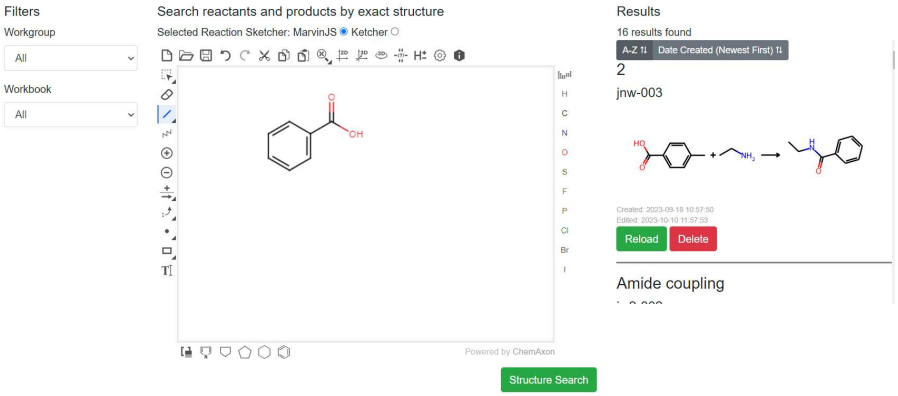


Information about the solvent guide can be found by pressing the “About the Solvent Guide” button.

Search

The navigation bar provides a link to the ‘Search’ functionality.

The user can search for structures and find all reactions from the workbooks they belong to which contain this structure. It is possible to filter the search by workgroup or workbook.



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.