



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.

The screenshot shows the AI4Green web application interface. At the top, there is a dark navigation bar with links for Home, Demo, Solvent Guide, and Workgroup. On the right side of the navigation bar, there are buttons for Help and a user profile dropdown for SamB. Below the navigation bar, a large light gray banner displays a welcome message: "Welcome to AI4Green, SamB!". Underneath the message, it states "AI4Green is an Electronic Laboratory Notebook built around encouraging green and sustainable chemistry." and provides two buttons: "Learn more" and "Quickstart Guide". Below the banner, the page is divided into two main sections. The left section is titled "Please select a Workgroup to get started" and contains a dropdown menu labeled "-Select Workgroup-", followed by four buttons: "Proceed to Workgroup" (green), "+ Join Existing Workgroup" (blue), "+ Create Workgroup" (blue), and "Workgroup Membership Summary" (blue). The right section is titled "News Feed" and shows a message "No news items to show!". At the bottom of the page, a footer contains the text "Last update 18/01/2023", links for "Hazard Disclaimer | Privacy Notice | Twitter", and the note "Hazard data sourced from ECHA references on PubChem".

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.

Development-Workgroup

User Type: Principal Investigator

Change Workgroup

Manage Workgroup

Manage Workbooks

Choose a Workbook to view or create reactions

Development-Workbook

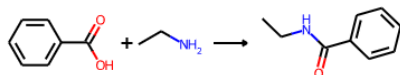
+ New Reaction

Your Saved Reactions

A-Z Date Created (Newest First)

Amide Coupling 1

Description of reaction.



2022-07-21 23:02:55.140833

Reload

Delete

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

Home Demo Help Manage Account Notifications Solvent Guide Workgroup Logout

Manage Workgroup

Workgroup Name: Development-Workgroup

Overview Requests

Name	Email	Actions
Principal Investigators		
Pat Inglis	PI@mail.com	↓ PI to SR Remove from Workgroup
Senior Researchers		
Sam Reed	SR@mail.com	↑ SR to PI ↓ SR to SM Remove from Workgroup
Standard Members		
Susan Matthews	SM@mail.com	↑ SM to SR Remove from Workgroup

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.

Reaction Builder

Please sketch or upload your reaction to begin

The screenshot shows the Marvin JS Reaction Builder interface. At the top, there is a prompt: "Please sketch or upload your reaction to begin". Below this is a toolbar with icons for file operations (save, open, print, etc.) and drawing tools. The main drawing area is a large white rectangle containing the Marvin JS logo and the text "Marvin JS by ChemAxon". To the right of the drawing area is a vertical menu with chemical symbols: H, C, N, O, S, F, P, Cl, Br, I. Below the drawing area are icons for different reaction types and the text "Powered by ChemAxon".

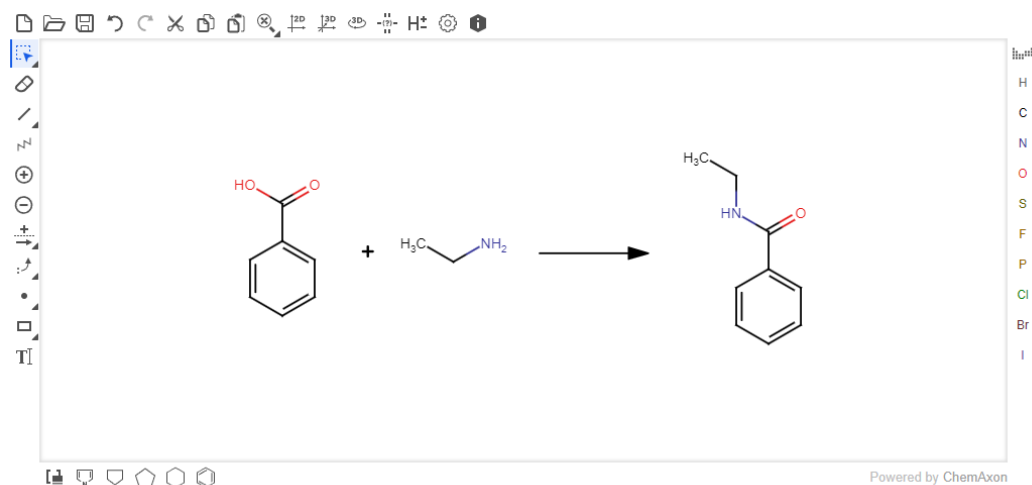
Example

Submit

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.

Reaction Builder

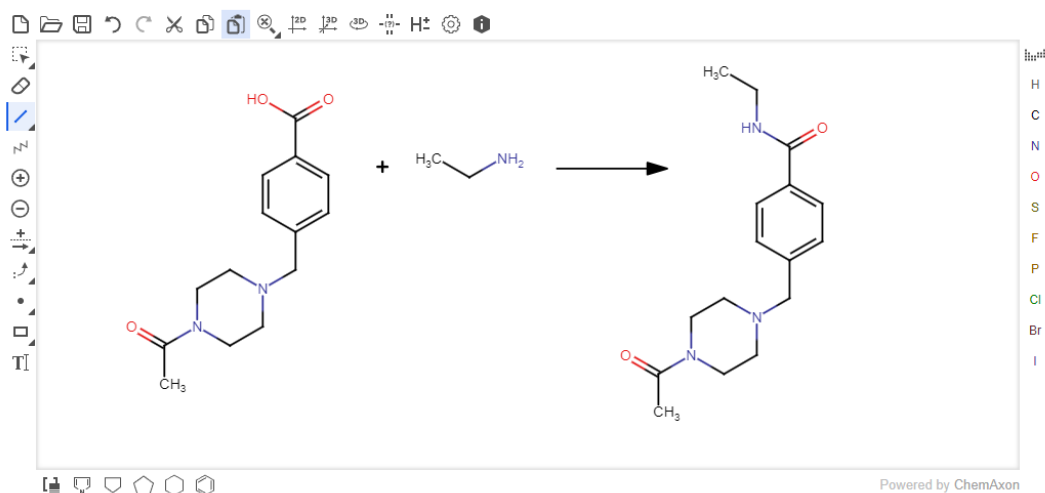
Please sketch or upload your reaction to begin



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’.

Reaction Builder

Please sketch or upload your reaction to begin



Example

Submit

Reactant 1 not in database.

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

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

No	Reactants	Limiting Reagent?	Mol.Wt	Density (g/mL)	Conc. (M)	Equiv.	Amount (mmol)	Volume (mL)	Mass (mg)	Physical Form	Hazards
1	Benzoic Acid	<input checked="" type="radio"/>	122.12	-	-	<input type="text" value="1"/>	-	-	<input type="text" value=""/>	<input type="text" value="-select-"/>	H315-H318-H372
2	Ethylamine	<input type="radio"/>	45.08	-	-	<input type="text" value=""/>	-	-	<input type="text" value=""/>	<input type="text" value="-select-"/>	H220-H319-H335

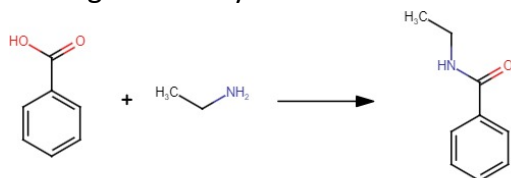
Catalysts/reagents

Solvents

Product

3	N-Ethylbenzamide	<input checked="" type="radio"/>	149.19	-	-	-	-	-	<input type="text" value=""/>	<input type="text" value="-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".



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

Hazards	Hazard Rating	Exposure Potential	Risk Rating
1 H315 Causes skin irritation, H318 Causes serious eye damage, H372 Causes damage to organs through prolonged or repeated exposure	VH	L	H
2 H220 Extremely flammable gas, H319 Causes serious eye irritation, H335 May cause respiratory irritation	H	H	H
3 H225 Highly Flammable liquid and vapor, H302 Harmful if swallowed, H318 Causes serious eye damage, H331 Toxic if inhaled, H335 May cause respiratory irritation	VH	M	VH
4 H228 Flammable solid, H315 Causes skin irritation, H317 May cause an allergic skin	VH	L	H

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.

Sustainability (CHEM21)							
Solvents	Safety	Temp °C	Elements	Batch/flow	Isolation	Catalyst	Recovery
Ethyl acetate	H1	20	+500 years	Batch	Column	No catalyst	--select--
	Atom Efficiency	Mass Efficiency	Yield	Conversion	Selectivity		
	22.0	10.7	74	90	82		
Standard Protocols:							
<input type="checkbox"/> Cyanide	<input type="checkbox"/> HPLC	<input type="checkbox"/> Mass Spec	<input type="checkbox"/> Pyrophorics	<input type="checkbox"/> Microwave			
<input type="checkbox"/> Diazotisation	<input type="checkbox"/> Hydrogenation	<input type="checkbox"/> Peptide Synthesis	<input type="checkbox"/> Ozone	<input type="text"/>			
<input type="checkbox"/> Free Radicals	<input type="checkbox"/> Liquid Ammonia	<input type="checkbox"/> Peroxides	<input type="checkbox"/> Sealed Tube	<input type="text"/>			
Disposal of Waste Materials:							
<input type="checkbox"/> Non-Halogenated Solvent	<input type="checkbox"/> Halogenated Solvent	<input type="checkbox"/> Specialist Container	<input type="checkbox"/> Sink with Excess Water				
Spillage Procedure:							
<input type="checkbox"/> Standard Spill Response	<input type="checkbox"/> Other Spill Response (Give details on unattended experiment board)						
Other Risks, controls, containment, location and PPE.							
(Hazardous by Products, Exothermic reactions, The need to inform others of risks, Lab and hood number.)							
<input type="text"/>							
Hazard categorisation given GLP and other controls specified							
Hazard Potential to cause harm	<input type="radio"/> 1. Slight <input checked="" type="radio"/> 2. Serious <input type="radio"/> 3. Major	Risk Category (A-D) <input type="radio"/> A (10-27)	Risk Score HxRxC				
Risk Likelihood of exposure	<input checked="" type="radio"/> 1. Low likelihood <input type="radio"/> 2. Possible <input type="radio"/> 3. Frequent Occur	<input type="radio"/> B (6-9)	<input type="text" value="2"/>				
Consequences Who will be affected	<input checked="" type="radio"/> 1. Individual <input type="radio"/> 2. Local Labs <input type="radio"/> 3. Building wide	<input type="radio"/> C (3-5) <input checked="" type="radio"/> D (1-2)					
Signed:							

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.

AI4Green User Manual – 01/2023 – 1.4

03/02/2023, 14:57
127.0.0.1:5000/report_data_getDevelopment/Workgroup2/Development/Workbooks/Incheset

test
Owner: PI_Dummy

Created: 2023-01-18 13:01:43 (GMT+01:00)
Last updated: 2023-01-18 13:01:43 (GMT+01:00)

#	Reactants/catalysts/reagents	Mol.Wt	Density (g/mL)	Conc. (M)	Eqivs.	Amount (mmol)	Volume (mL)	Mass (mg)
1	Benzic Acid	132.12			1	0.02	0.00	2
2	Ethylamine	45.08			2	0.03	0.00	1.48

Solvents		Volume (mL)	
3	Acetic acid		2

Product	Mol.Wt	Theoretical Yield (mg)	Unreacted	Product Mass (mg)	% Yield
4	N-Ethylbenzamide	149.19	2.44	0.1	62

Hazards	Hazard Rating	Exposure Potential	Risk Rating
1 H315 Causes skin irritation, H318 Causes serious eye damage, H372 Causes damage to organs through prolonged or repeated exposure	H	L	H
2 H228 Extremely flammable gas, H314 Causes serious eye irritation, H330 May cause respiratory irritation	H	M	H
3 H228 Flammable liquid and vapor, H260 May be corrosive to metals, H314 Causes severe skin burns and eye damage	H	M	H
4 H302 Harmful if swallowed	M	M	M

Sustainability (CHEM21)

Solvents	Safety	Temp °C	Elements	Batch/flow	Isolation	Catalyst	Recovery
Acetic acid	H	100	C, H, O	Batch	Distillation, 1 atm, 0	Controlled reagents	Not recovered catalyst
	Atom Efficiency	Mass Efficiency	Yield	Conversion	Selectivity		
	85.2	82	98	98	98		

Standard Protocols:

<input type="checkbox"/> Cyanide	<input type="checkbox"/> HPLC	<input type="checkbox"/> Mass Spec	<input type="checkbox"/> Pyrophorics	<input type="checkbox"/> Microwave
<input type="checkbox"/> Diazotization	<input type="checkbox"/> Hydrogenation	<input type="checkbox"/> Peptide Synthesis	<input type="checkbox"/> Ozone	<input type="checkbox"/>
<input type="checkbox"/> Free Radicals	<input type="checkbox"/> Liquid Ammonia	<input type="checkbox"/> Peroxides	<input type="checkbox"/> Sealed Tube	<input type="checkbox"/>

Disposal of Waste Materials:

<input type="checkbox"/> Non-Halogenated Solvent	<input type="checkbox"/> Halogenated Solvent	<input type="checkbox"/> Specialist Container	<input type="checkbox"/> Sink with Excess Water
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Spillage Procedure:

Standard Spill Response Other Spill Response (Give details on unattended experiment board)

Other Risks, controls, containment, location and PPE.
(Hazardous by Products, Exothermic reactions. The need to inform others of risks, Lab and hood number.)

Print 2 pages

Destination Save as PDF

Pages All

Pages per sheet 1

Margins Default

Options
 Headers and footers
 Background graphics

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

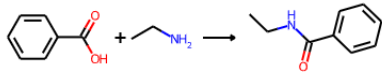
Export Data

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.


Your Saved Reactions

A-Z ↕ Date Created (Newest First) ↕

Amide Coupling
DW1-003



2023-02-09 14:20:05.802127

Reload  Read-only reaction created by SM_Dummy

Amide-3
DW1-004

Export Reaction Data

Export as CSV Export to 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

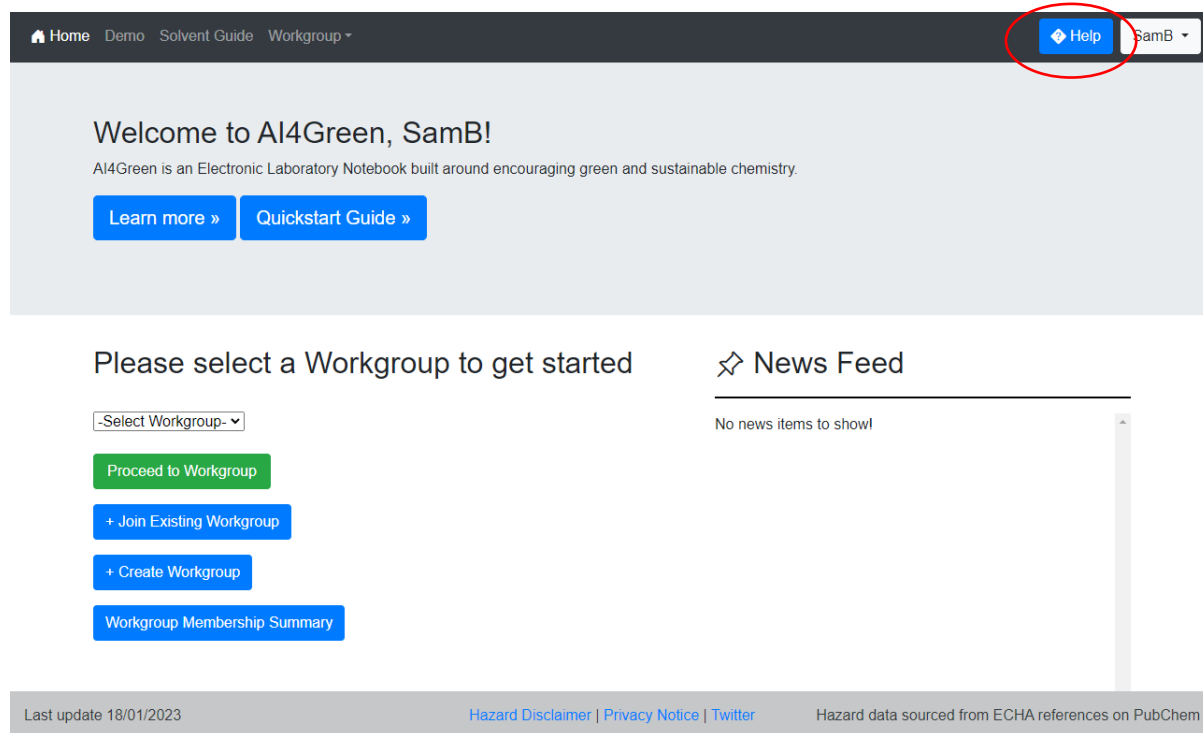
The solvent guide can be accessed from the top navigation bar or while building a reaction. The latter option will preload the solvent selected into the solvent guide.

No	Reactants	Limiting Reagent?	Mol.Wt	Density (g/mL)	Conc. (M)	Equiv.	Amount mmol	Volume mL	Mass mg	Physical Form
1	Benzoic Acid	<input checked="" type="radio"/>	122.12	-	-	<input type="text" value="1"/>	-	-	<input type="text" value=""/>	<input type="text" value="-select-"/>
2	Ethylamine	<input type="radio"/>	45.08	-	-	<input type="text" value=""/>	-	-	<input type="text" value=""/>	<input type="text" value="-select-"/>
Catalysts/reagents										
<input type="text" value="Add new reagent to database"/>										
Solvents										
<input type="text" value="Add new solvent to database"/> <input type="text" value="mL"/>										
3	<input type="text" value="Acetic acid"/>	<input type="button" value="Solvent Guide"/>			-			<input type="text" value=""/>		<input type="text" value="-select-"/>
Product										
<input type="text" value="Desired Product?"/> <input type="text" value="mmol"/> <input type="text" value="mg"/>										
4	N-Ethylbenzamide	<input checked="" type="radio"/>	149.19							<input type="text" value="-select-"/>

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.



The screenshot displays the AI4Green web application interface. At the top, a dark navigation bar contains links for Home, Demo, Solvent Guide, and Workgroup. On the right side of this bar, a blue 'Help' button with a white question mark icon is circled in red, and a user profile dropdown for 'SamB' is visible. Below the navigation bar, a large light gray banner welcomes the user 'SamB!' and provides a brief description of AI4Green as an Electronic Laboratory Notebook. Two blue buttons, 'Learn more »' and 'Quickstart Guide »', are positioned below the banner. The main content area is divided into two columns. The left column, titled 'Please select a Workgroup to get started', features a dropdown menu labeled '-Select Workgroup-' and four buttons: 'Proceed to Workgroup' (green), '+ Join Existing Workgroup' (blue), '+ Create Workgroup' (blue), and 'Workgroup Membership Summary' (blue). The right column, titled 'News Feed', shows a heading with a star icon and a message 'No news items to show!' above a vertical scrollbar. At the bottom of the page, a gray footer contains the text 'Last update 18/01/2023', links for 'Hazard Disclaimer | Privacy Notice | Twitter', and the note 'Hazard data sourced from ECHA references on PubChem'.