Empowering scientists to make sustainable choices

AI4Green is a suite of software that helps chemists to:

* manage their research data
* work more efficiently
* collaborate securely around the world
* be more sustainable

Royal Academy of Engineering

AI4Green: the intelligent ELN for sustainable discovery

Core functionality and AI tools
tested in lab environments at several institutions
hosting 471 users and 837 reactions

Publicly hosted at https://ai4green.app

Source code under the AGPL-3.0 licence

Boobier, S., Davies, J.C., Derbenev, I.N., Handley, C.M. & Hirst, J.D. AI4Green: An Open-Source ELN for Green and Sustainable Chemistry. *J. Chem. Inf. Mod.*, **2023**, *63*, 2895

Functionality

✓ Track and optimise reaction conditions

✓ Assess and reduce environmental impact

✓ Collaborate seamlessly and securely with colleagues

✓ Make data-driven decisions

✓ Automatically retrieve hazard codes

✓ Automatic data backup

✓ Enhanced search functionality

✓ Generate professional-standard COSHH assessment matrices

✓ Automatically calculate molar amounts

✓ Quickly search reactions by structure

✓ Draw reactions in an integrated chemical sketcher

✓ Join workgroups by QR code

✓ Electronic signature for reaction approval

A partially complete Reaction Table

№	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	0.06	0.00	7	Dense solid	H315-H318-H372
2	Ethylamine	○	45.08	-	-	6	0.34	0.00	15.5	-select-	H220-H319-H335
	Catalysts/reagents Add new reagent to database										Add Reagent
3	Name or CAS Number		-	-	-	-	-	-	-	-select-	
	Solvents							mL			Add Solvent
4	Name or CAS Number	Solvent Guide			-			-		-select-	
	Product	**Desired Product?**					mmol		mg		
5	N-Ethylbenzamide	◉	149.19				0.06		8.55	-select-	H302

Users are directed to provide information (highlighted in red). Reagents, solvents and novel compounds can be added / removed. Some information, *e.g.*, molecular weight, hazard codes, automatically populated from PubChem.

PubChem OPEN CHEMISTRY DATABASE

Part of the Summary Table

	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	L	M
3	H225 Highly Flammable liquid and vapor, H301 Toxic if swallowed, H311 Toxic in contact with skin, H315 Causes skin irritation, H319 Causes serious eye irritation, H331 Toxic if inhaled, H370 Causes damage to organs	VH	M	VH
4	H302 Harmful if swallowed	M	L	L
			Risk Rating:	VH

Sustainability (CHEM21)

Solvents
Methanol

Safety	Temp °C	Elements	Batch/flow	Isolation	Catalyst	Recovery
VH	40	+500 years	Batch	Column	Catalyst or enzyme	Recovered catalyst

Atom Efficiency	Mass Efficiency	Yield	Conversion	Selectivity
89.2	31	82	86	95

→ Information about the hazards of the reactions

→ Various green and sustainability metrics and considerations

Green metrics calculator

Automatic calculation of holistic reaction sustainability metrics including solvent sustainability, atom economy, and mass efficiency.

Informed by the CHEM21 consortium, our integrated sustainability metrics help researchers make decisions about their reaction conditions

➔ more sustainable outcomes and reduced environmental impact.

Solvent substitution

Solvent Guide

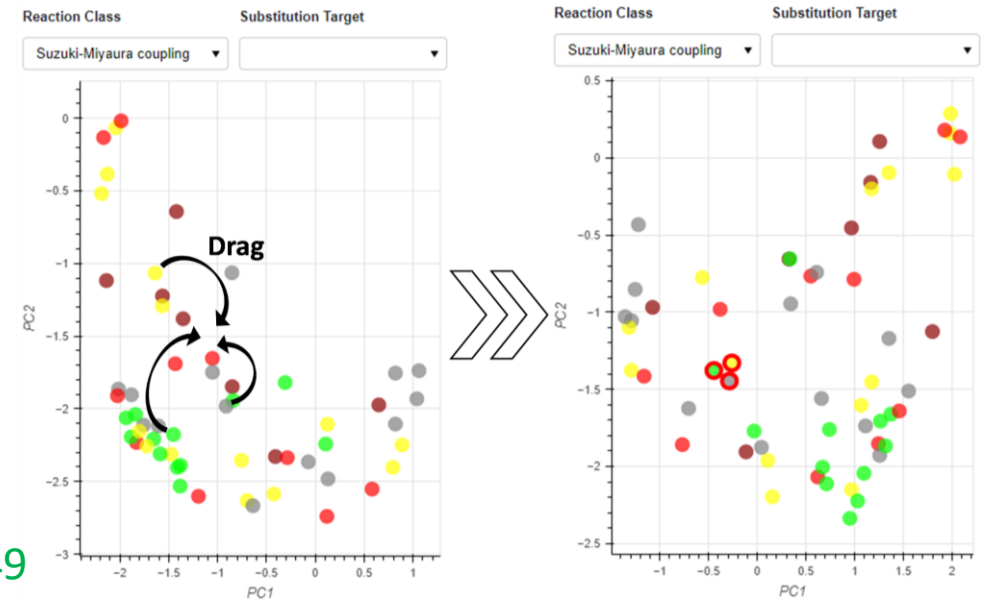
Interactive flashcards provide visual rationale for the sustainability of a solvent and recommended greener alternatives.

Make more informed choices about solvents with our simple customisable and colour-coded system.

Solvent Surfer

Interactive tool for exploring and comparing different solvents based on their physical properties and environmental impact for different reaction classes.

Drag points to impart your own knowledge on the tool and tailor for your specific use case to identify greener alternatives.

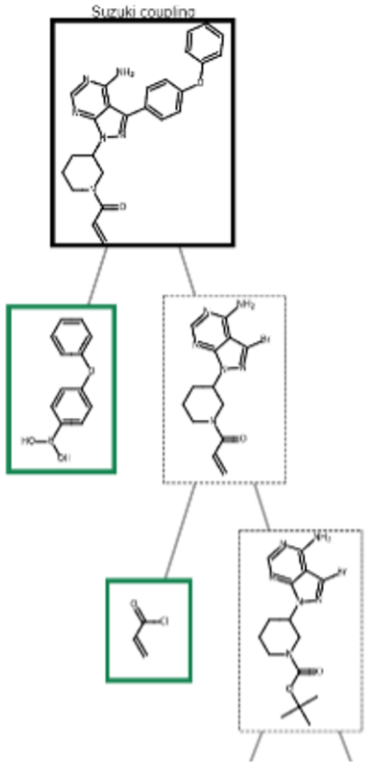


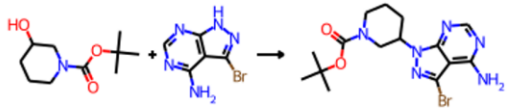
Boobier, S.; Heeley, J.; Gärtner, T.; Hirst, J.D. Interactive Knowledge-based Kernel PCA for Green Solvent Selection. *ACS Sus. Chem. Eng.*, **2025**, *13*, 4349

Retrosynthesis planning

AI-powered retrosynthesis route planning tool with condition prediction to design more sustainable synthetic routes.

Rapidly generate and analyse potential synthetic pathways considering factors, such as:
solvent sustainability
atom economy
reaction safety.





Condition Set 1

	Conditions & Sustainability
Likelihood Score	0.63
Temperature (°C)	19
Solvent	Tetrahydrofuran
Reagents	Triphenylphosphine, CC(C)OC(=O)N=NC(=O)OC(C)C
Catalyst	None
Element Sustainability	50-500 years
Atom Economy	45.2%
Safety	H225, H319, H335, H351

Step Analysis	1	2	3	4	5	6
Solvent						
Temperature						
Catalyst						
Element Sustainability						
Atom Economy						
Safety						
Weighted Median						

Adjust Sustainability Metric Weightings

Solvent Default
Temperature Default
Catalyst Default
Elements Default
Atom Economy Default
Safety Default

Blackshaw, T.M.; Davies, J.C.; Spoerer, K.T.; Hirst, J.D. Enhancing Monte Carlo tree search for retrosynthesis. *J. Chem. Inf. Model.*, **2025**, *65*, 6537

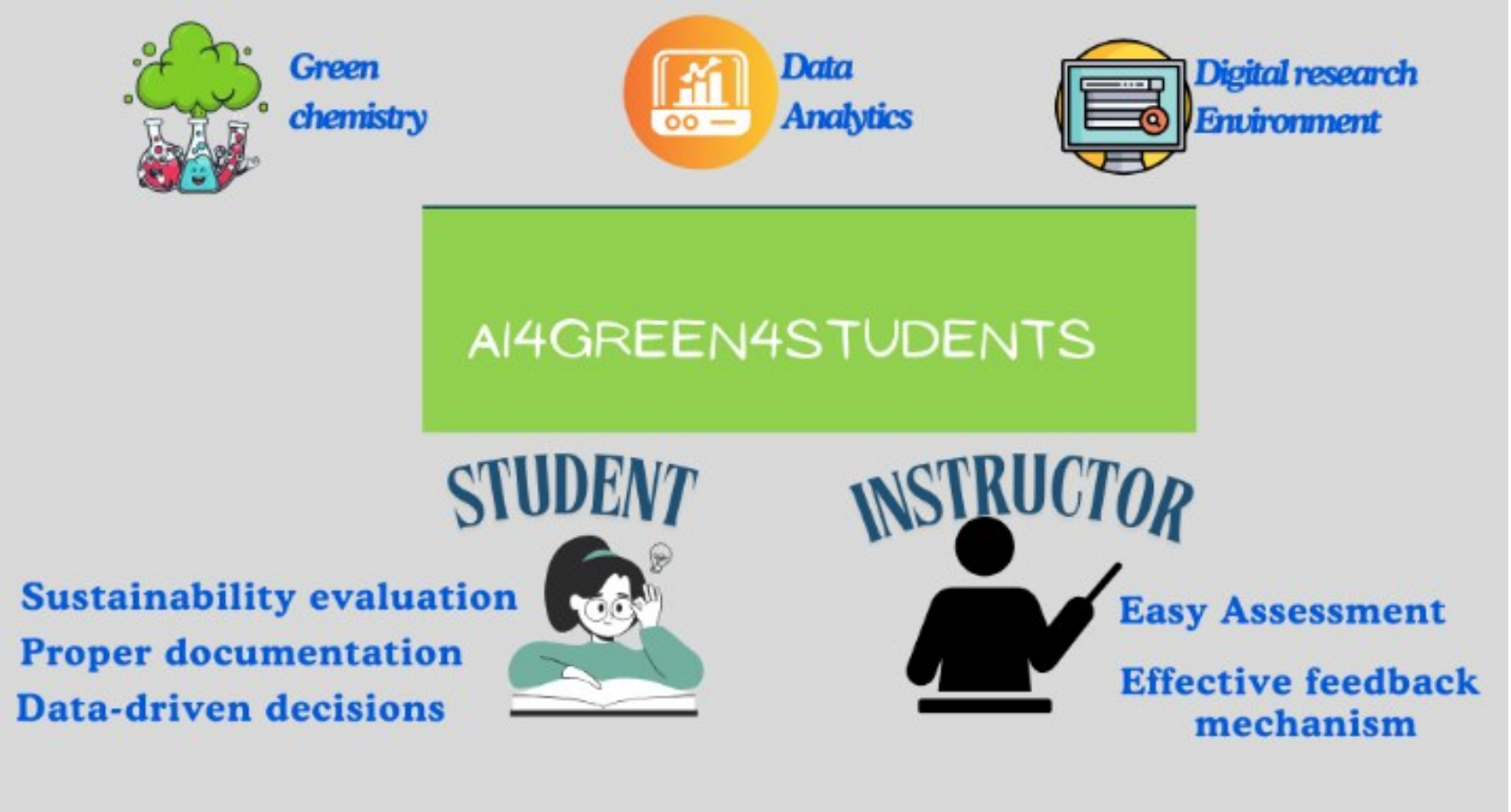
User feedback

“Our research team at Strathclyde has been one of the early adopters of the AI4Green, and it is helping us to monitor and improve the sustainability of our chemistry”

“I would recommend this to my peers as it is a much more streamlined approach to handling data, and it can be retained and accessed easily in the future”

“It's a great tool for everyday work and have encouraged other members of our research group to join, and it has significantly streamlined the planning/write-up process”

AI4Green4Students



Nwafor, P.; Gurung, S.; van Krimpen, P.; Schnaubert, L.; Jolley, K.; Pearman-Kanza, S.; Willoughby, C.; Hirst, J.D. AI4Green4Students: Promoting sustainable chemistry in undergraduate laboratories with an electronic lab notebook. *J. Chem. Educ.*, **2025**, *102*, 2720−2731

AI4Green4Students

AI4Green4Students designed specifically for use in undergraduate laboratories.

Students must input their own hazard codes and molar calculations which are checked automatically by the system.

It teaches students data management, green chemistry principles, and software skills.

The assessor view provides a superior ability to monitor and provide feedback on their students work.

Functionality to add new experiments

The platform includes:

- Simplified interface for educational settings
- Learning resources
- Teacher management tools and assignment features
- Focus on fundamental green chemistry concepts
- Green chemistry metric calculators

https://ai4g4s.app/

AI4Green: the intelligent ELN for sustainable discovery

Freely available for academics

Interested in AI4Green?
Scan the QR code
to send us an email!

AI4Green4Students: teaching for a sustainable future

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