Science AMA Series: We designed a method to quantify how "green" a chemical is; We're Jane Murray and Samy Ponnusamy, Ask us anything!

Millipore-Sigma [1] and r/Science AMAs[1]

[1]Affiliation not available

April 17, 2023

Abstract

Our recently published paper in the ACS Sustainable Chemistry & Engineering journal describes a quantitative assessment tool to evaluate chemicals and chemical processes against the 12 Principles of Green Chemistry, using generally accepted industry practices and readily available data sources. This tool, called DOZN, provides a consistent framework for measuring and communicating what's "greener" about the products labeled as "greener alternatives" and is robust and flexible enough to encompass a diverse product portfolio, from biology to chemistry to materials science. So, feel free to ask us anything about this tool and how it's currently being implemented at MilliporeSigma, or how you can apply it in your organization. We'll be back at 1:00 PM Eastern Time (10 am PT, 6 pm UTC) to answer your questions, ask us anything! Dr. Jane Murray: I am the head of Green Chemistry for the Life Science business of Merck KGaA, Darmstadt, Germany, which operates as MilliporeSigma in the U.S. and Canada. I have a background in chemical research—having completed my Ph.D. at the University of York, where I researched green oxidations of organosulfur compounds using hydrogen peroxide. I am a member of the American Chemical Society's Green Chemistry Institute, Chemical Manufacturer's Roundtable, the Royal Society of Chemistry and the American Chemical Society. Dr. Ettigounder "Samy" Ponnusamy: I am the Green Chemistry Fellow with the Life Science business of Merck KGaA, Darmstadt, Germany, which operates as MilliporeSigma in the U.S. and Canada. In this role, I manage and expand new green business opportunities, as well as research and develop greener alternatives—including spearheading the DOZN tool that we'll be talking about on this AMA. I have more than 30 years of experience managing new product developments—from bench scale through product launch—with many products showing sustained growth over time. I earned my Ph.D. from the University of Madras and am the co-author of 30 related scientific articles and holder/co-holder of seven patents. Edit: We forgot to include the link to the paper: http://pubs.acs.org/doi/pdfplus/10.1021/acssuschemeng.6b02399 Edit 2: We'll be back in an hour to begin answering but wanted to share a link to the 12 Principles of Green Chemistry that we referred to at the top - https://www.acs.org/content/acs/en/greenchemistry/what-is-green-chemistry/principles/12-principles-of-green-chemistry.html Edit 3: Hi everyone, thank you for all of the questions. We'll be sticking around until 2:30 EST to answer questions, so keep them coming. If you're interested in learning more about MilliporeSigma's program, you can go to www.sigma.com/greener Edit 4: Thank you everyone for the great questions! This was both of our first times on Reddit and we appreciate the informative and engaging discussion - hopefully you did as well. We're sorry if we weren't able to get to your question but we hope to be back here sometime soon. If you have time, feel free to take a look at the links we shared above and throughout our answers. If you'd like to see an example of our DOZN scoring for a real product, you can see it here: http://www.sigmaaldrich.com/catalog/product/sigma/a7005 If you have any other feedback or questions, please continue to post. We'll continue to revisit this thread and may even answer a few more questions. Thank you again!

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REDDIT

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MILLIPORE-SIGMA R/SCIENCE

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If you have any other feedback or questions, please continue to post. We’ll continue to revisit this thread and may even answer a few more questions. Thank you again!

READ REVIEWS

WRITE A REVIEW

Just to help me wrap my head around this, what common chemicals are "most green" and "least green", why?

CORRESPONDENCE:

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[communistmilk]

That’s a big question that doesn't have one simple answer but one beginning point is hazard. This is can be a good initial indicator. Minimal or no hazard can start you in the direction of greener and products with more hazardous hazardous can be less green. We use the 12 Principles of Green Chemistry to help us determine greenness. The greenest chemicals minimise the use and generation of hazardous substances, require minimum resource and energy consumption. (JM)

Are there any misconceptions of what is considered 'green' that you'd like to set right? Did your research result in any unexpected results in terms of the 'green'-ness of certain chemicals?

[Fog_Terminator]

One misconception is that things are “green” - we use the term greener because it’s really challenging in this space to have something be truly green. I think when we started we didn’t quite understand the potential of the tool to help us understand how changes we made impacted the environmental footprint of the product we were reengineering. Ultimately the lesson learned is be open to surprises and thankful when they help guide you to something you didn’t expect. (SP)

How do you feel about advertisements and branding of products on the market, currently?

My understanding is that 'green,' 'sustainable' and other marketing terms can be widely used without any science or regulating body ensuring that those claims are sound.

[Tremor_Sense]

We developed DOZN in response to the need for a scientifically substantiated way to quantitatively assess the “greenness” of a chemical. Previous “green” marketing may only concentrate on one aspect eg resource use whilst ignoring the hazard impact to the environment. The 12 Principles of Green Chemistry, developed by Anastas and Warner, look at the entire environmental impact of a chemical including resource use, energy efficiency and hazard impact. These 12 principles were adopted by the Green Chemistry Institute(GCI) at the American Chemical Society (ACS). Our DOZN system was developed based on the 12 principles of green chemistry to provide a comprehensive assessment on the relative greenness of product or process. Our approach and algorithms were also independently verified by a 3rd party. (JM)

Do you worry that your work will be misused for 'green-washing', with companies manipulating things for the appearance of being greener?

I'm thinking about things like the can of aerosol citrus cleaner I have that claims to be both "aerosol-free" and "chemical-free". When I press the button it literally dispenses a chemical aerosol - maybe d-limonene, I think.

Is your tool designed to be used within industry for decision making by those designing products and processes, or for consumers to inform themselves?

[madsci]

What you bring up is an interesting point. This is why we press for transparency and data driven outcomes. This helps mitigate the potential for green-washing. Will we be able to stop every instance - probably not. But by making data the core of our system you can start invoking transparency which makes it a lot more work to green-wash and diminishes benefit. The tool is really used for industry and

decision making for those creating/designing/researching to help minimize the footprint from the beginning. (SP & JM)

Hello Dr. Murray and Samy. Thank you for taking the time to share your work with us.

- What does DOZN stand for? And roughly how does it work?
- What makes a product green in your mind? The term gets used a lot, but I'm not aware of a single agreed upon definition.
- How well, in your opinion, do current efforts at green products and technologies achieve what they claim?
- What's the most counter-intuitive result you've found in your research. For example, everyone thinks "X is green and Y is not, but it's actually the other way around"
- Are there deceptive tactics that companies use to appear environmentally friendly that consumers should look out for?

PapaNachos

The correct answer is DOZN™ - the ™ is simply a trademark, that in some systems doesn't get superscripted; The name acknowledges the 12 Principles of Green Chemistry upon which the system is based. Greener products' environmental footprint should be much smaller or nil. Our viewpoint is that our work is an iteration forward. You'll see us use the word greener because it's step change improvement and we don't want to mislead consumers by using green as an absolute. Data is important to use to back up what we state - without data/research we don't want to make any claims that can't be backed up. One example we saw in the early days of our work was a product that was a carcinogenic chemical in a recyclable package and calling it greener is not a green product at all. MilliporeSigma developed DOZN to address all these tactics used in the market and provide proof why the materials are considered greener or not. We hope that we can create a tool that pushes the industry forward regarding transparency and intentionality to provide scientists with accurate data that helps make informed decisions. (JM & SP)

Could you define "green" as it pertains to this tool?

gwdope

We use the industry accepted 12 Principles of Green Chemistry. These were developed in 1998 by Warner and Anastas and reduce or eliminate the use or generation of hazardous substances, minimise resource use and increase energy efficiency.

Are there substances you already know this method will not calculate accurately?

elheber

Our method would work well as long as one inputs all the manufacturing information, GHS and SDS information and provide accurate results. It's important to have the data - it drives the system and makes the quantification possible.

Is your method based on the concept of life cycle analysis? If not, how are they different?

atchoe

LCA often does not incorporate all 12 principles of green chemistry. Our DOZN system does. We discuss the differences in detail in our ACS publication http://pubs.acs.org/doi/abs/10.1021/acssuschemeng.6b02399.

One important thing to note about LCA's - while extremely thorough, they're often difficult, time consuming and expensive to complete. We approached this challenge to create a cost and time effective solution that moved us in a direction toward LCA but that was achievable considering the scale of products that we have.

Do you consider super critical CO2 as a green chemical solvent?

puretree

Yes, for some applications super critical CO2 can reduce large volumes of solvent usage. One thing we find is that a lot of the times it's really an "it depends" situation and doesn't always apply.

Could one or both of you describe the path(s) you took to reach the positions you have in your scientific career(s) today? I am a 4th year undergrad interested in graduate studies in biochemistry, and I am trying to collect the stories of those with experience to help me decide what is best for me. Thanks!

organizedcarbon

First and foremost thank you for considering graduate studies in biochemistry. To be frank, initially you will go through some rough roads but ultimately it will be rewarding and you will have a sense of accomplishments.My experience during my graduate work was very motivated with my friends and peers and at industry my success was purely due to customer driven challenges. (SP)

I think it's important that you enjoy the work that you do. I believed in the goals of my PhD, loved the City I studied in and was surrounded by great friends - this helps you through the tough days in the lab. I chose to work in Industry as I always enjoyed seeing Science applied in the real world. In my current role I'm lucky to still get to work with inspiring academics and be involved with cutting edge technologies. (JM)

Thanks for your time doing this AMA. Some people asked about labeling "green" chemicals and I ask the opposite question. Do you think "not green" chemicals should be labeled with that info?

umgajonormal

Our DOZN system can be applied to all chemicals and will assign them a score out of 100. Therefore less green chemicals will be readily identified (through a higher score) and can be readily compared to lower scoring "greener" alternatives. You can also think of GHS as a very effective visual warning system for products that are less green.

That's great and will help genuinely concerned consumers.. but do you think it will actually reach a point where some chemicals will be so not-green that they would actually be forced to be removed from the market because of your findings? Meaning might you expose something so toxic that the regulation agencies actually remove it from sale?

exotics

This is a great point - it's already happening and not because of our tool - as more safety data comes out, governmental organizations are starting to either regulate or ban materials from use. This actually provides a great opportunity to find better alternatives for these products, encourage innovation and create a market opportunity. Organisations are given time to find safer alternatives. If you look at the ECHA/ REACH framework, chemicals are typically listed as a "substance of very high concern" for some time before there is pressure to replace.

We are actively introducing alternative chemicals where restrictions are increasing eg our new solvents Cyrene is a greener alternative to DMF and NMP solvents that are under increasing regulatory pressure. At the end of the day if scientists ask the question that you've ask it has entered into their consideration process and that's a huge part of the battle.

Is there a standard (world wide) for green chemicals or is each country able to decide what's green in their eyes and for their environment?

Also what are the most practical methods of choosing green chemicals for the everyday consumer?

Thank you!!

shinatree

There's not a single standard available as of today this is why we created DOZN to begin that conversation with the hopes of moving to a framework that can be widely accepted to help make informed decisions.

For consumers this task is difficult but there are several initiatives and companies which are working on ingredient and labeling transparency to make this task simpler for the consumer. It's still a work in process. (SP)

Hello and thank you for taking the time to share this and answer questions. One of the hardest things to determine for me as a consumer is the efficacy of various green products. I know that I have purchased greener alternatives on a number of occasions that worked so terribly I had serious buyers remorse and wished I had gone for the less green original.

To me this is a serious problem because I WANT to be green(er) but if being green means a higher cost to me i.e. the product (say a paint solvent) cost 125% of the original AND requires 300% additional labor then the actual cost is 425% of the original.

I will generally engage in the greener alternative anyway out of moral concerns BUT here's the rub. I often hear other consumers complain that they won't buy 'that green shi*' because it doesn't work. I think that creates a fundamental trust issue where 'green' translates to 'doesn't work'

I appreciate the work that you're doing and I hope that it has it's intended impact. Sincerely. I am also curious to know, to what extent does this tool account for efficacy and how will it help to engender trust in green chemistry?

circumflexiblation

Our approach to greener is mainly driven by cost parity or savings for the consumer - we aim for the win/win to give customers solutions that work. (SP)

Performance is critical. Our new solvent, Cyrene, demonstrates that a safer greener product can also

provide superior performance (when compared to NMP in the production of Graphene). We work closely with Academics to introduce more such innovative green products to our portfolio. Ultimately, if it doesn't work we haven't done our job which means adoption won't happen and then we've created more waste. (JM)

Hello, thank you for taking the time to answer questions! As someone who has only recently begun working in the field of TEA/LCA it is great to see how passionate people are in the field.

I have a couple of questions if that is okay:

Rapid assessment is a major focus in the LCA/TEA community currently, with a focus on developing streamlined but reliable & replicable methods for analysis.

Do you see DOZN as a tool that can provide such analysis?

You speak of using a broader data set than that used in an LCA, how do you quantify the qualitative factors? How can you ensure that this doesn't allow for bias when used by others?

dipdipderp

That is not only our hope but intention. While we recognize that it's not as thorough as an LCA it's usable and efficient data in decision makers hands to hopefully make more informed choices.

The data set that is used is driven by GHS information which helps diminish things like bias as it is fixed. There are certain elements, like pollution prevention which are more difficult to quantitate but our goal was to start somewhere and then iterate forward in collaboration with the global scientific community to continue to move the tool forward. (JM)

How green is plastic used in packaging (bottles, wraps, etc.)?

asmj

This is improving as more bio-based alternatives become available. See for example Paperfoam's Frima ice cone tray or Tipa's bio-based fully compostable plastic packaging alternatives. (JM)

Thank your for doing this AmA. How do you plan to label a product in terms of green-iness? Furthermore for whom will be a need and what was the initial reason to develop this method?

thermokilometer

Thank you for your interest. The 12 Principles of Green Chemistry, developed by Anastas and Warner, are widely recognised and accepted by Scientists. These 12 principles were adopted by the Green Chemistry Institute(GCI) at the American Chemical Society (ACS). We developed our DOZN system to quantitatively assess chemicals, using the 12 principles of green chemistry. The DOZN tool assigns a chemical a score (from 0-100) so that Chemists can quickly and easily assess the "greeness" of a chemical, 0 being the most desired. We saw a gap in the market of being able to quantify greenness and wanted to begin the work to address this - we believe that this is just the first step in a longer process but a good start to engage in conversation and iterate our framework forward. (SP)

What chemicals do people consider green that surprisingly are not? What chemicals do people treat like villains that are surprisingly green?

Opcn

Misconceptions happen when only one area of "greenness" is considered eg focussing on resource use but not toxicity could result in labelling a recycled but toxic chemical as "green". The DOZN system takes a more holistic approach by utilising the 12 Principles of Green Chemistry and therefore prevents this from happening. (JM)

Thank you for taking the time to do this AMA! I have a few questions.

1.Have any plans been made or are underway to require your rating on chemical labels?

1. I am a chemistry major who is about to start applying for chemistry PhD programs. It has been difficult for me to narrow down programs since I am still unsure of what I want to research (I am interested in inorganic chemistry and catalysis and possibly nanotechnology). How did you know which school/program was right for you?
2. After graduating, how similar was your research to your thesis?
3. What made both of you venture away from working in the lab and want to work more in the business end of the industry?

IworshipCthulhu

The ratings are currently accessed via our website. You can see an example of this here: http://www.sigmaaldrich.com/catalog/product/sigma/a7005

I choose my PhD based on my interest in the subject area.

I choose to work in industry as I enjoyed seeing Science applied in the real world. (JM)

Is water a green chemical?

joshcamas

Yes, water is considered the safest solvent. (JM)

What products do you recommend/discourage?

AronBhalla

We are introducing more bio-based chemicals to address our environmentally unsustainable dependence on petroleum based feedstocks. Just because it's bio-based though doesn't mean that it's necessarily better though so you have to be mindful that it's not a regrettable substitution. Once again - the answer is it depends. (JM)

As an Indian I feel really proud to see you doing very well, Thanks for the AMA. I live in Madras (Chennai now) too and the question is for the both of you

1.What are some of the parameters you have that determine whether the product is green or not? 2. And why DOZN?

NKrishnaStark

Thanks. Our DOZN system utilizes all aspects of the 12 Green Chemistry Principles to find out relative greenness of product or processes. DOZN system is simple, reliable, robust and economical. DOZN is a play on 12 - just minus the e! :) (JM & SP)

Can DOZN be used to inform and improve current life cycle assessment (LCA) data and tools?

kimmersly

This is a great one - LCA's are challenging and expensive. We debated this and figured that we'd bankrupt the company if we tried to do LCA's for all of our products. So if you don't attempt at all then it's a miss. So, in our viewpoint, this is the continuation of a conversation about quantification and how we can continuously improve our approach - so short answer, we think so!

Products like "Green works" sell an idea of a green product with no backing information, what is best used to combat this in an industry that can create its own falsehoods?

stripesndredlights

DOZN which requires readily available information like manufacturing inputs, GHS and SDS information drives home the requirement of data and quantification. Our process is simple, transparent and data-driven helping us to start providing more information so informed decisions can be made.

Question to Dr.Samy: What is your advice to young Indians who are pursuing a career in Biotechnology? You seem to be from South India (I bet Tamil Nadu). What social problem in India do you think needs an immediate scientific solution?

darksoysauce

Thank you for your question. I believe opportunities are abundant but one has to be willing to adapt to the continuous change in Biotechnology (SP)

This is very interesting. Thanks for putting this on a platform where the regular folks like myself can learn. My question is a few parts. Is there a database of chemicals to search and learn about? Is this a program where I can input info from the manufacturer or MSDS sheet to calculate it's greenness? And last, can this quantification be measured on a 1-10 scale and universally be labeled on products that fall within particular guidelines? Thanks again and I hope I got in the AMA!!

normball

Very soon you will be able to interact with DOZN - while it does require some base information it will give you a starting point. Our scale goes to 100 with a lower score being more desirable. Some of our products now have a DOZN score on the product detail pages so you can see the improvements that have been made.

We are still working on how we display the information, but you can see an example how we identify a greener product here: http://www.sigmaaldrich.com/catalog/product/sigma/a7005 (SP)

Thank you so much for doing this AMA!

I have a couple questions:

1) Do you expect this approach being eventually modified to support chemists to estimate greeness during product development? In a way making estimates from the lab on what the performance of the product will be in production?

2) While the application of a ranking facilitates decision making, do you think this could potentially lead to misinterpretations and misuse of results by companies?

3) with this method companies can set system boundaries based on data availability, how effective do you think the method is in conveying data gaps, analytical choices and assumptions?

4) One much discussed topic in LCA is uncertainty. This method doesn't seem to account for that. What is your opinion on the inclusion or exclusion of uncertainties?

5) Have you already identified potential case studies that you would like to work on to compare LCA to this method?

6) I had another question but I forgot :) ...

Thanks again!!

edit: separated two questions

EnviroLeontief

Absolutely - this is DOZN 2.0 which we expect to be ready in 2018. We needed a starting point but also realize that it was very limited. Now that we've gained experience we're able to better understand how we expand the tool to take into account process rather than just product.

There's always a possibility of misinterpretation but the data aspect and transparency helps to mitigate this - we continue to look at how we can continue to reduce that potential as we iterate the tool forward.

Our tool uses a fixed set of data however the potential of uncertainty always exists and accounting for that is a challenge that we're still working through - ideas are always welcome!

We have a strong base of products that we could do a comparison but haven't invested the money in that because of the cost - but a great suggestion of a next step for a gap analysis.

If you remember just let us know ;) (JM)

Is the measurement of how green a chemical is dependent upon its renewability? Or more so how toxic/harmful it can be?

I ask because in a lot of industrial processing, we use chemicals which are very toxic, but none of which I wouldn't consider green when handled properly and recycled.

On another note on the topic of being green, where do you fall on the GMO versus organic food industry scale?

mworhatch

Both, DOZN includes all aspects of the 12 principles of green chemistry in measuring the greener score. So factors like renewability and toxicity factor in to the scoring methodology.

Is this a purely negative scale, or does it include positives?

I.e. does it rate chemicals only on how harmful they are to the environment or does it leave space for them to be beneficial?

If so, how common is that as an output of human activity?

Froztwolf

DOZN tool provides the scientists to screen and find out the relative greenness of product or process and employ in their application. Also DOZN incorporates all aspects of the 12 Principles of Green Chemistry. Our tool provides needed information for the customers to screen both positive and negative impacts based on the score. So it's not just negatives - some of the characteristics are positive - like renewables. (SP)

Is your software based on LCA? What makes it innovative or different from an other LCA software like Sima Pro or Gabi?

forgot_name_again

LCA's often does not incorporate all 12 principles of green chemistry. Our DOZN system does. We discuss the differences in detail in our ACS publication http://pubs.acs.org/doi/abs/10.1021/acssuschemeng.6b02399. One important thing to note about LCA's - while extremely thorough, they're often difficult, time consuming and expensive to complete - even with some of the tools mentioned. We approached this challenge to create a cost and time effective solution that moved us in a direction toward LCA but that was achievable considering the scale of products that we have. (SP)

Do you think your efforts will have any effect on what is being used in households and by companies? Frankly, it seems like only certain companies even care an ounce about how environmentally friendly their product is, as long as it doesn't harm their economic success.

It's really nice that someone is working on the problem on the science/chemistry level. But if it doesn't simplify or save resources immediately, it will be overlooked by the ones actually producing and using the chemicals.

arduheltgalen

Our work isn't just limited to providing data - it's then actively engaging with industry and researchers to implement. We're beginning to engage with personal care companies, textile and apparel companies, etc. It's a slower process but we see progress happening. In addition to helping customers assess the greenness of a chemical we are actively adding more greener alternatives to our catalogue. In some instances the greener alternatives can offer improved performance (eg the use of our new solvent Cyrene in the production of Graphene). So I think the easier we make it for our customers to switch then the more likely they are to do so. A number of our chemicals (eg Performance Materials products used in electronics applications) do end up in households. As consumers ourselves we are driven to make these products as "green" as possible. Another aspect of this is the choices that consumers make with their purchasing decisions - that trend has definitely affected companies decision to make greener products. (SP & JM)

what is the final equation that determines the score? and what is the scale of this score (is there a cap)?

assman4000

There are twelve equations (one for each principle) and then we group them into three categories (Reduced Resource use, Increased Energy Efficiency and Reduced Human & Environmental Impact) and get the aggregate score from 0 to 100 (0 being the most desired). You can see the equations by checking out the paper http://pubs.acs.org/doi/pdfplus/10.1021/acssuschemeng.6b02399.

Very nice work, I love seeing green chemistry concepts gaining traction.

How do you see your work extrapolating to the palladium/ligand catalyzed couplings that have become so indispensable in the industry?

Typical_mann

In partnership with Dr Allan Watson at the University of Strathclyde, we have looked at the solvents that are employed in these reactions. We found we could replace reprotoxic DMF with safer, bio-based Cyrene in Sonogashira couplings. We initially focussed on solvent usage in these reactions as it accounts for more than half the waste in a typical Pharmaceutical process. We also offer Lipshutz Surfactant- this enables palladium catalysed cross-couplings to be carried out in water at room temperature. (JM)

So now a days people are using concepts like green and healthy living to make other consumers feel as though chemicals are bad. Are there any ways your program helps combat the fear of chemicals?

kittenbeauty

Our system quantitatively assesses the greenness of a chemical using industry accepted criteria. By assigning a score consumers can quickly understand the "greenness" of a chemical. A chemical with a low score would indicate that it had limited environmental impact (resource and energy) and minimal toxicity (to both humans and the planet). Our results are also verified by a 3rd party. A component of this is education and there is still a lot of work to be done. (JM)

Is the method susceptible to abuse?

kinxen

The simple answer is no. With the data requirements transparency is harder to mask. (SP)

Why do reaction conditions/safety play a role in the "greenness" of a process? From my perspective, many reactions performed under milder lab conditions require more steps, solvents, and catalysts versus the industrial processes where a well-engineered reactor designed to run at extreme pressures and temperatures can do it in one fell swoop.

nick_t1000

DOZN system utilizes all parameters in the calculation (reaction conditions, temperature, pressure, number of steps, solvents, catalysis, etc.) to generate the "greenness" score. So there are considerations taken from a variety of angles - as hazard consideration is one of the 12 Principles this is why it's included. (SP)