AI 4 Science Discovery Network+

AI4SD Interview with Dr Nessa Carson
06/12/2021
Online Interview

Michelle Pauli
Michelle Pauli Ltd

12/08/2022

Humans-of-AI4SD:Interview-36

AI4SD Interview with Dr Nessa Carson
Humans-of-AI4SD:Interview-36
12/08/2022
DOI: 10.5258/SOTON/AI3SD0233
Published by University of Southampton

Network: Artificial Intelligence and Augmented Intelligence for Automated Investigations for Scientific Discovery
This Network+ is EPSRC Funded under Grant No: EP/S000356/1

Principal Investigator: *Professor Jeremy Frey*
Co-Investigator: *Professor Mahesan Niranjan*
Network+ Coordinator: *Dr Samantha Kanza*

Contents

1 Interview Details **1**

2 Biography **1**

3 Interview **3**

1 Interview Details

Title	AI4SD Interview with Dr Nessa Carson
Interviewer	MP: Michelle Pauli - MichellePauli Ltd
Interviewee	NC: Dr Nessa Carson - Syngenta
Interview Location	Online Interview
Dates	06/12/2021

2 Biography

Figure 1: Dr Nessa Carson

Nessa Carson: 'My advice to early career researchers? Do good work and talk about it'

Nessa Carson received her MChem degree from Oxford University, before completing postgraduate studies in catalysis and organic methodology at the University of Illinois at Urbana-Champaign. She started in industry as a synthetic chemist for AMRI, then moved within the company to run the high-throughput automation facility on behalf of Eli Lilly in Windlesham, working across both the discovery and process chemistry arenas. She then worked in process development using automation at Pfizer. Nessa started at Syngenta in 2020, working in automation, reaction optimization, and data management. She maintains a website of useful chemistry resources, https://supersciencegrl.co.uk.

In this Humans of AI4SD interview she discusses the speed and power of automation in the lab, the importance of data management, getting a job via Twitter and her advice for early career researchers.

3 Interview

MP: What's been your path to where you are today?

NC: I always liked chemistry, even when I was a little kid before most people knew what chemistry was! I like reading, and I read a science book from the library that told the stories of what famous scientists did from around the Middle Ages onwards. I thought it sounded cool because they're all just playing really, aren't they? But they got to discover new things and find out about how the world works, and hopefully make new things that make the world better. When I first did organic chemistry, I liked it because it seemed very ordered: there's a set of rules and you think that everything follows the rules. Within a year of learning chemistry, you find out that nothing follows the rules and chemistry is just chaos!

I now work in reaction optimisation and automation chemistry, where I guess I am trying to get some order from the chaos, mapping out reactions in chemical space. My background is in synthetic organic chemistry, so I had never planned to go into automation, but during my work in industry, I got the opportunity to move into an automation laboratory and to run it from my department. I'd never have guessed that it would be possible for me to do it with the background I have, but after a week of solid training and some on-the-job learning, it was clearly suited to me.

One thing that appealed to me is the fact that you're doing things very fast — everything's quick and you need to be responsive to different things. Another aspect of it is that high-throughput automation chemistry is a really social job. That meant I got to go around the department and talk to everyone, because I work across projects rather than being tied to a particular one.

MP: What made you choose to go into industry rather than staying in academia?

NC: I had been in grad school in the States for three and a half years, and I expected a PhD in my group would probably have been about seven years. That's how it is in organic chemistry in the States. But after that time, I felt like I was stagnating a bit in terms of learning, and learning was the one thing I really wanted to be doing. I think I would have been quite bored carrying on with my PhD, so I'm glad I got my Masters instead, and went into industry where the amount of learning went straight back up again.

MP: What are you working on currently?

NC: I'm honestly working on a little bit of everything! I'm in the lab a lot less than I used to be, and doing more data work: I'm working on some cool projects to do with data management.

One of the things I'm working on is reaction optimisation. It's incredible how much of a difference it can make to projects in pharma and ACRA-Chem. If someone has a reaction that isn't working, they basically give it to me, and I ought to be able to fix it very quickly. Usually I do this by running a hundred reactions and seeing what works best within the constraints and guidelines for the experiment. With that, you can map out data very quickly. Typically in a high-throughput lab, I was doing 10 plates a week, which is really effective. It's great the amount of money you can save and the amount of chemical space you can map: it really couldn't be done any other way.

MP: How does this work change how science is done?

NC: One thing that is going to change a lot is a different aspect of automation, which involves connecting up data and hardware. Having everything talk to each other is great, but not in the way that if one part breaks down, everything breaks down. Instead, when one part of a system or a workflow knows the previous parts that have been done, it makes things go much faster. That could have a huge impact on discovery chemistry as well as process chemistry. It would mean that less time is wasted on the routine manual work and more is spent on the expert manual work: it would free up the time to do the clever things that make science happen!

MP: What kinds of challenges do you face in this work and what has surprised you?

NC: One challenge is the fact that good equipment can be expensive, and trying to get that funding can be problematic sometimes. Luckily, the equipment I'm working with is fast, but it depends on how much people are willing to invest in your lab.

In terms of what surprised me, at first, I was really surprised by how much you can do; ten 96-well plates in a week is loads! What also surprises a lot of people is the variety of chemistry you can do. When people first hear about automatable chemistry, they think about the library synthesis side of things. But with reaction optimisation, there isn't much you can't do if you have the kit: gas reactions, cold reactions, pressure reactions, they're all perfectly fine. The only things I wouldn't want to use are explosives, but I'm sure you can do it with them. It's surprising how much you can do.

MP: What issues do you come up against with data management, and how do you manage these?

NC: If you start off with a project that hasn't been designed with data in mind, then it's really difficult to get people to use and understand it properly. When you're running 96 reactions at a time, for example, you won't collect the data effectively if you don't store it effectively. Then in two years' time, if somebody else wants to run a similar reaction, if you haven't stored the data effectively, they won't have a way to quickly read about them and understand what's going on — they have to start from a blank slate. You're also completely unable to use something like machine learning if you haven't stored data in a sensible way. You want your data to be both human-readable and machine-readable.

One really important thing is whenever you start a new workflow, you should build in the sensible data workflow right from the beginning. Then, when you have new users, you need to tell them: "This is how we have to do it." It's a lot easier to start that way, than to convince people who don't care that much about data after they've been doing things their own way. It's important to have that kind of data mindset right from the start of a project. You don't need to bore everyone with every detail; it can be as simple as telling people: "Writing your file names in this way is useful for machine learning and other people looking at your data. This is how we do it." Most people don't have a complaint with that.

MP: Where have you found important scientific communities?

NC: Twitter has been so useful. Getting my first job, for example, I had posted on Twitter that I was looking for jobs and someone fantastic, who I'd never met in real life at the time,

got in touch with me and told me about a job. It hadn't been what I was thinking of, but he persuaded me to apply for it. I did and I got the job, and the guy from Twitter became an awesome mentor of mine.

There's also a community on Discord that came from chemistry Twitter, which is a little more private. There's probably around 200 people in it now, and there are loads of different channels which provide people with spaces to talk about things that are positive, as well as when things aren't working out for them. It's been really useful.

I also just love conferences: I genuinely go to about one a month. It's really great to have this network of people that you can meet and hang out with.

MP: What advice would you give to early career researchers in your field?

NC: If you want to do social media and want to connect with other researchers, then it can be really great. But if you don't want to do it you don't have to: it's not worth your time trying to put energy into that kind of thing.

Going to conferences can also be a little difficult as an early career researcher, especially if you don't have the funding. But there are sometimes ways around that. If you reach out to the organisers, they're sometimes able to offer a discounted registration, so it's definitely worth trying.

For me, all the good things have come from working with other amazing scientists. Some of them I met on Twitter, some of them I met at conferences, some of them I've worked with. If you're looking for people who want to use science to make the world better, there are definitely some around.