Artificial Intelligence and Augmented Intelligence for Automated Investigations for Scientific Discovery

AI3SD Interview with Dr Mark Warne
01/02/2021
Online Interview

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Humans-of-AI3SD:Interview-18

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Title	AI3SD Interview with Dr Mark Warne
Interviewer	MP: Michelle Pauli - MichellePauli Ltd
Interviewee	MW: Dr Mark Warne - DeepMatter Group
Interview Location	Online Interview
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2 Biography

Figure 1: Dr Mark Warne

Dr Mark Warne: 'Chemists are a bit like artists, the equivalent of a Michelin-starred chef"

Mark Warne is Chief Executive Officer of DeepMatter Group. He is widely recognised in the UK and international life sciences sector, having spent almost 10 years at IP Group Plc, a leading intellectual property commercialisation company, where he led the healthcare team and managed a portfolio of £330m of net assets in 2016/2017. He has a PhD in computational chemistry, an MSc in colloid science and a BSc in chemistry, all from the University of Bristol.

In this Humans of AI3SD interview he discusses the digitalisation of chemistry, the challenge of reproducibility, changing mindsets and why chemists aren't really like the Swedish Chef...

3 Interview

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

MW: I did my undergraduate degree, master's and PhD in computational chemistry, and started as an early career researcher in a business based in Cornwall that was part of a US NASDAQ-listed computational chemistry company. I spent eight years there, initially as a scientist and ending up as managing director of the business, which was ultimately sold on to a giant conglomerate. I then spent 10 years investing in early stage life sciences for IP Group, starting in technology life science propositions but moving into digital health and applications of data and real-time data collected from local sensors in the digital health field.

After 10 years with IP Group, I decided to go back into industry and took the opportunity to lead what is now DeepMatter. It is a business focused on the digitisation of chemistry, applying many of the things that I saw in the field of digital health but in a pre-clinical setting. It was an area that looked like it had been untouched by technology development and wasn't taking advantage of things like cloud-based computing and the distribution of local sensor arrays.

At DeepMatter we built a platform collecting data, structuring it to improve the productivity of the research process of chemists across the board. Whether from industry or academia, it aims to help them discover better, be more efficient in the way that they work and, ultimately, to improve the health and safety and environmental factors in labs.

MP: Was chemistry particularly behind other sciences?

MW: I think so, and for a couple of reasons. The first is that there were very established workflows in chemistry and so to motivate people to collect data differently, to structure that data differently, is a high bar. Changing people's behaviours is a hard thing to do. Secondly, chemists like to go into the lab to do chemistry. They don't want to spend all their time doing a type of data science. Computational chemists might think differently but, ultimately, a synthetic organic chemist or an analytical chemist wants to do what they are trained to do. Putting a high digital burden on them is difficult. Also, chemists think of themselves as artists. I always think of them in that light, the equivalent of a Michelin-starred chef. They create and so the idea that what they do could be digitised, or improved by an element of digitalisation, is probably an effort. In addition, data collection has historically been very much geared towards a protocol, which people tend to write after an experiment rather than before. So, collecting data post-hoc is not necessarily a massively useful thing to do. You really need to have intent before you go into the lab. All chemists have intent. No one goes in the lab like Swedish Chef, just throwing ingredients into a bowl. But while they think about what they're going to do, very few of them write it down before they go in. And that means that you don't ultimately know what did change when you were in the lab or the impact of any changes that you may have made. That's an embedded mindset that is difficult to shift.

Secondly, and this is also quite hard, you run the risk of looking like you are blaming chemists for failure in the lab, whether it's the environmental conditions or using the wrong reagents or having the wrong information to start with or general inaccuracy from the chemist – that sort of burden is quite a hard thing for the chemist to accept. As a student, I was as guilty as any chemist of going into a lab with a hangover. I'm sure my chemistry was worse on those days than on the days when I was performing better. Maybe it's the other way around. Who knows? In contrast, in other sciences, such as biology, there's always been more of a culture of attributing failure to something you can't control, such as the behaviour of cells.

Most of the challenges in chemistry have come about as a result of behavioral change difficulties, which are more to do with nature, how chemistry is taught and how chemistry ownership within the chemistry community has been based.

MP: It sounds like quite a lot of barriers there to be overcome, particularly around behavioural and cultural mindsets. How do you go about shifting that?

MW: Patiently. The way to lift those barriers is to provide benefit back to the users from day one. In any environment you will not change people's behaviour by simply foisting a product on them. So you do it in stages; you provide tools to them that make their job a little bit easier, a little bit more efficient, a little bit more fun. That's the sort of learning that you might take from consumer applications of digital technologies. Had I presented you 15 years ago with a mobile phone and told you that you were going to do your banking on it, most people would have laughed but now we do everything through that lens of technology. Taking technologies that the users are familiar with and providing them with a little bit more all the time is a really useful thing to do.

The second way to change bigger behavioural mindsets, like writing a protocol before you go into the laboratory rather than afterwards, is to find a real pain point for the user community and introduce a way of overcoming that pain point. A good example is that every chemist who goes into a lab these days has to complete health and safety forms and it's a real pain to complete those little forms. So if you could make it a one-click environment, it reduces time and burden for the individual. Then suddenly you do have a protocol in advance, but you need to find a way of making sure that's automatically embedded into the way that they're performing chemistry in the lab and recording data.

Then you need to demonstrate value from the applications that you're using quite quickly. A really good example is that we have a collaboration with Novartis and they embedded the technology platform that we use to collect video data on the inside of a round bottom flask. Now, no one that I am aware of has yet quantified the importance of the visual changes going on inside a round bottom flask for outcomes and reactions. But what we know is the team at Novartis are particularly focused on environmentally sustainable chemistry. We know that that means using aqueous solutions with surfactants rather than organic solvents. I'm sure anyone who's got even basic chemistry will know that surfactants tend to result in colour change and opacity change. And suddenly the feed that you take out of a video camera could become very valuable. We need to show the correlations between traditional outcomes and these novel surveys and collect that in real time. All those things will engender the change, but it doesn't happen overnight.

MP: What about benefits such as enhanced reproducibility, collaboration?

MW: Reproducibility is really important. As a scientist, I really care about it. In particular, I think in teaching, in academic research and anywhere where you make reagents and then make them over and over again, the ability to reproduce designs and demonstrate the benefits of making certain changes is a really powerful tool.

It's interesting though, when we talk to early-stage research and pharma, they really couldn't care less about reproducibility because what they care about is making a new drug, and does whatever they make first time round have a therapeutic effect on the essay that they're testing? Of course, if the drug or the compound works and then they can't remake it, that may change their view as they move down the stream. We see a big drive from the contract research organisations and the lifestyle integration providers who make a compound one year and then two years later are unable to embed the knowledge or re-synthesise the compound at a scale that they were interested in for whatever reason previously.

A really precise digitally encoded recipe is invaluable but I think reproducibility is a means to an end for us. The drivers we see from the people who buy our products are a preference for productivity gain or the ability to discover a new molecule rather than reproducibility per se. But if the system is not reproducible, the whole thing falls apart.

MP: What does digital chemistry or the digitisation of chemistry mean to you? And what is it not?

MW: For us, the digitisation of chemistry is the encoding of the chemical knowhow in people's heads and in people's hands into a form that can be used by another person, be it an expert or someone less experienced to reproduce the work that's been done previously to ensure a good transfer of knowledge.

Once upon a time, you probably could have stood two feet or less from another scientist and watched the precision of their hands and what they do in their reaction and learned from it. But that's going to be less and less common and so digital technologies are going to collect and structure that data in such a form that someone should be able to reproduce it.

If I give you a Jamie Oliver cookbook and ask you to reproduce a perfect souffle, there'll be information in that cookery book that will assume a degree of knowledge on your part or will not impart every piece of information that might be useful to you. Whereas if I play you a video of the same thing, you'll see that when Jamie Oliver says "fold", what fold actually means. If you can embed that sort of knowledge or collection of data into something computational, that allows you to reproduce it.

For us, having got that caucus of knowledge of both positive and negative outcome data, it's important to collect the failures as well as all the successes. We now have a very large dataset of not just the reactions with outcomes, but also the time course stage as well. That then lends itself to machine learning applications.

As for AI, I think that we can provide a better, safer, improved, more efficient journey for the chemist and some of that will be done through some degree of autonomy by using robotics. If a reaction isn't going correctly, do you really need to stand there and turn up the dial or whatever it might be when actually a piece of robotics can do that?

But at the same time, chemistry is inherently a dangerous business. We work with nasty, explosive chemicals. There are things that we don't want robots to do for us because they're not safe. And so at the very end of the scale, I don't think we're moving towards a world where local chemistry will be done robotically. I think we'll be moving to a world where certain applications can be done more efficiently, allowing chemists to focus on what they're good at, which is design, and put more distance between chemists and dangerous chemicals.

MP: What elements of your work in relation to digitalising chemistry has surprised you?

MW: I think what has surprised me the most is the lack of correlation between experience and precision in the lab. We look at lots of chemists doing lots of chemistry and we collect and restructure that data. The variation between a top-tier superstar chemist and a highly inexperienced chemist doesn't correlate with their training, their experience or who they are. Only if you guide them down very specific paths do you move towards a high level of reproducibility.

One of the fears will always be that with the more reproducibility you embed, do you hamper innovation? I don't believe that's true. I think we will reduce more errors than hamper innovation. What we might be seeing is less serendipitous discoveries because, ultimately, as people see the value in being guided towards successful outcomes, you don't produce those possibly serendipitous mistakes in quite the same way.

MP: How has Covid-19 affected your work?

MW: It has generated a lot more interest in digital methods. People are looking for disruptive solutions to the way they operate their labs. They're obviously having to work fundamentally differently from the ways they used to. Lab occupancy fell from 100% to 30%, maybe even lower in some cases, at the start of the pandemic. There are many different practices being employed and digital technologies allow people to access data differently, share data differently and work together differently. Digitalisation was already a trend but Covid has accelerated the adoption of these technologies and over the next couple of years we'll see them really embed properly.