Artificial Intelligence and Augmented Intelligence for Automated Investigations for Scientific Discovery

AI3SD Interview with Professor Jonathan Goodman
14/07/2020
Cambridge, U.K.

Professor Jeremy Frey
University of Southampton

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Network: Artificial Intelligence and Augmented Intelligence for Automated Investigations for Scientific Discovery
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Contents

The AI for Science Network interviewed Jonathan Goodman before his online talk for the Network on InChI: The IUPAC international chemical identifier.

1 Interview Details

Title	AI3SD Interview with Professor Jonathan Goodman
Interviewer	JGF: Jeremy Frey - University of Southampton
Interviewee	JG: Professor Jonathan Goodman - University of Cambridge
Interview Location	Cambridge, U.K.
Dates	14/07/2020

2 Biography

Figure 1: Professor Jonathan Goodman

Jonathan is a Professor of Chemistry at the University of Cambridge, and Director of Studies of Chemistry at Clare College, where he also serves as the Academic Dean. His research focuses on experimental and computational chemistry, analysing organic reaction mechanisms, interpreting analytical data and investigating computational chemical toxicology. He is also secretary of the Subcommittee on the IUPAC International Chemical Identifier and has developed the Reaction-InChI (RInChI): an InChI-based identifier for chemical reactions.

3 Interview

JGF: Jonathan, what or who first excited your interest in Chemistry?

JG: I grew up in Middlesbrough near the Teesside chemical factories and in North Yorkshire near medieval blast furnaces. One of my grandfathers was a chemistry teacher, and the other worked for ICI (Imperial Chemical Industries) where my father also worked, so chemistry was always a central part of the world around.

JGF: Jonathan, what was your PhD research area? Why did you choose this topic?

JG: My PhD, with Ian Paterson, focussed on boron-mediated aldol reactions and was sponsored by Eli Lilley. This began as an experimental project and progressed towards computational analysis with the common theme of understanding organic reactivity and developing better transformations. I wanted to discover more about how molecules behave and react, and this project was an ideal way to do this as the reaction was new and exciting, I could study it using a variety of different methods, and I had a link with a pharmaceutical company which helped me see how these discoveries could be applied to create useful processes and molecules.

JGF: Jonathan, what did you do after your PhD? When did you decide to pursue and academic career?

JG: After my PhD, I did a post-doc with Clark Still at Columbia University, before returning to Cambridge where I have been ever since.

JGF: How did you become interested in computational chemistry?

JG: Whilst I was doing my PhD, I discovered that calculations could aid experimental chemistry. Computers were very slow at the time, compared with the resources we have today, and my first insight into computational organic chemistry was that reactions which are accessible to calculations are impossible to do in the organic laboratory, and vice versa. Fortunately, the boron-mediated aldol reaction, which I was studying experimentally, was one of the few exceptions to this rule, as the heart of the process involved just six atoms from the first row of the periodic table and seven hydrogen atoms and the reaction could be run in a variety of solvents with similar outcomes. The success of this joint use of experiment and calculation led to the investigation of much more complicated processes.

JGF: How would you distinguish between computational chemistry and chemical informatics?

JG: Computational chemistry begins with models of molecules, usually based on force fields or density functional theory, and uses these to investigate molecular structure and chemical reactivity. Chemical informatics begins with data, from every available experimental source and from all possible calculations, and extracts chemical understanding from these. Both are important for developing our understanding of chemistry and ability to design and to manufacture molecules.

JGF: How did you become involved in IUPAC and the InChI?

JG: Twenty years ago, Alan McNaught, who was president of IUPAC's Division VIII

(Chemical Nomenclature and Structure Representation Division), invited me to a meeting in Washington DC to discuss a proposal that IUPAC should be involved with a new structure representation standard developed by Steve Heller at NIST and called the IChI. Many committee meetings later this developed into the InChI that we use today.

JGF: Jonathan, what does being the Academic Dean involve?

JG: The University of Cambridge is a collegiate university, and each college within it provides undergraduate teaching. My role as Academic Dean at Clare College is to ensure that we have the right faculty members to keep the college running smoothly and to persuade them to devote some of their time to teaching as well as to research.

JGF: Jonathan, as secretary, what are your plans for the InChI IUPAC subcommittee?

JG: The IUPAC InChI subcommittee makes recommendations for the parts of the InChI project which are most deserving of support. If you have ideas for extensions to the InChI standard, or for new areas to which it could contribute, please let me know. If you would also like to develop these ideas, that would be even better!

JGF: How has COVID-19 affected your teaching and research?

JG: Teaching on-line works effectively, once everyone has got the technology is more or less under control and become used to tutorials being invaded by household pets. Everything needs additional planning and adjustment to make the best of these new conditions. Now that we are becoming accustomed to them, changing back will take some thought. I hope we will end up training students and each other even more effectively, because we have been obliged to try out alternative approaches. This should help us to think about the best ways of communicating and explaining chemistry.

Much of my research is done sitting in front of a computer. However, it is more interesting and fruitful to be able to meet people in person than to be restricted to on-line conversations and I look forward to being able to do more of this once we are through the waves of COVID-19.

JGF: How to you see the role of Artificial Intelligence in the future of Chemistry?

JG: Our current knowledge of molecular behaviour is limited by the amount of data we can acquire and analyse. There is a limit to the quantity and complexity of data that a human can assimilate. In principle, AI will make it possible to generate knowledge from datasets too large and too complex to analyse in other ways. This might enable us to discover exactly how difficult chemistry really is.