AI 4 SCIENTIFIC DISCOVERY

DECEMBER 16, 2022

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

FINAL REPORT 2018-2022

Final Report
Report Date: 16/12/2022
DOI: 10.5258/SOTON/AI3SD0271
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
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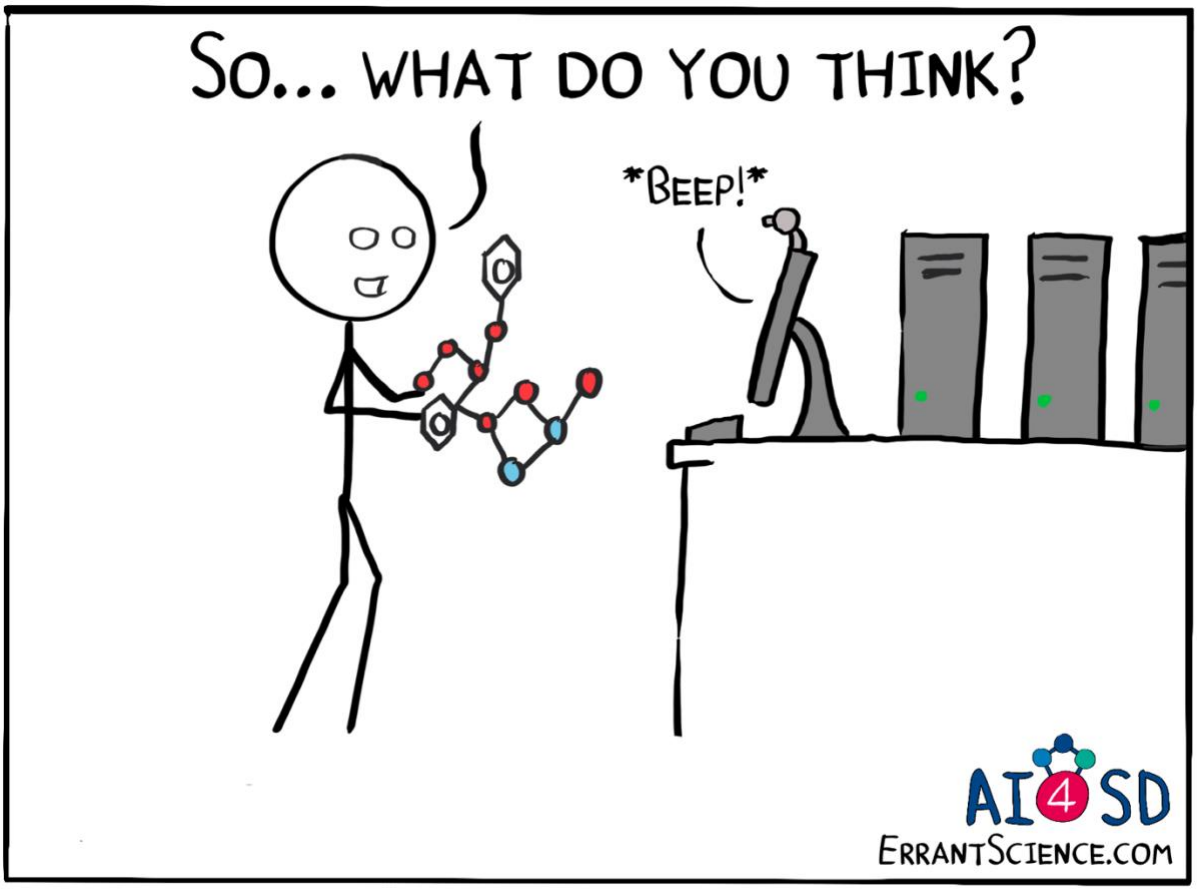

Engineering and Physical Sciences Research Council

AI4SD AI 4 SCIENTIFIC DISCOVERY

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1. Introduction

The Network has run for four very successful years between 2018-2022. Over these four years we created a community of over 1500 people and gained a strong social media presence, especially on twitter. We have funded 7 pilot projects, 15 interns and over 120 students to attend our machine learning summer schools, in addition to providing training to hundreds of other Network members through our Failed it to Nailed it and Skills4Scientists series. We were undeterred by COVID and took our Network activities online, doubling our membership over the summer of 2020 and bringing us a new array of international members where before we had been predominantly UK based, and since the return of physical events, we converted to a hybrid Network bringing together the best of both worlds for a mix of hybrid and virtual activities.

The Network has produced an immense number of resources, including 174 videos for our YouTube Channel and 52 reports across funded projects and events, in addition to supporting the publication of 19 peer reviewed journal and conference papers. The Network has also been heavily involved in other projects including supporting an Ethics for AI working group, and some collaborative projects with the Network of Networks group to run an Equality, Diversity, and Inclusion survey, and to write and compile a very comprehensive resource on how to run a Network which has been distributed to new Networks who were looking for guidance. Overall we feel that this Network has been very successful both in terms of impact and outputs.

This report provides a comprehensive overview of the Network. Section 2 details our membership statistics and growth, different social media and website accounts, and statistics on our events. Section 3 lists our outputs, Section 4 contains impact statements and collated feedback on our funded initiatives, and Section 5 describes our other outputs including our work with the Network of Networks.

2. Network Details

The Network was funded by EPSRC and hosted by the University of Southampton. Our primary aim was to bring together researchers looking to show how cutting edge artificial and augmented intelligence technologies can be used to push the boundaries of scientific discovery. Our initial focus was Design and Synthesis of Chemicals and Materials. Many of our events and initiatives were linked with these aspects, and we expanded our remit to run training events on data sharing, machine learning and to provide scientists with the range of required skills to work in the intersection of chemistry and computer science. This section details our different account details, membership, both in terms of the mailing list and social media and event statistics.

2.1. Website, Mailing List & Social Media

The Network has gained a strong web presence over the last four years, particularly with respect to Twitter and YouTube.

Table 1 shows the location of all the different Network websites and social media accounts that have been setup.

Table 1: Network Website, Mailing List and Social Media Accounts

Type	Link
Website	https://www.ai4science.network/
Mailing List	https://www.jiscmail.ac.uk/cgi-bin/webadmin?A0=AI4SD
Twitter	@AISciNet
Eventbrite	https://ai4sd.eventbrite.com
YouTube	https://www.youtube.com/channel/UCXOkV943dmo6rSiVlo7lsBw
LinkedIn	https://www.linkedin.com/company/ai4sd/
Instagram	@aiscinet
Facebook	https://www.facebook.com/AISciNet

2.2. Statistics

This section details membership and event statistics for the Network.

2.2.1. Membership

The Networks membership is defined by the mailing list, which currently has 1572 members. We also have several different social media accounts. Twitter has provided us with the most engagement, followed by YouTube despite this not being setup until 2020. Overall, the Network has shown steady growth in most of these areas. Table 2 shows the different membership numbers for the mailing list and the range of Network Social Media Accounts Figure 1 shows the membership growth over the last four years.

Table 2: Membership Statistics for the Network

Type	Numbers (Dec 2022)
Mailing List Membership	1572
Twitter Followers	961
Eventbrite Followers	384
YouTube Subscribers	767
LinkedIn Followers	120
LinkedIn Interest Group Members	50
Instagram	51
Facebook	13

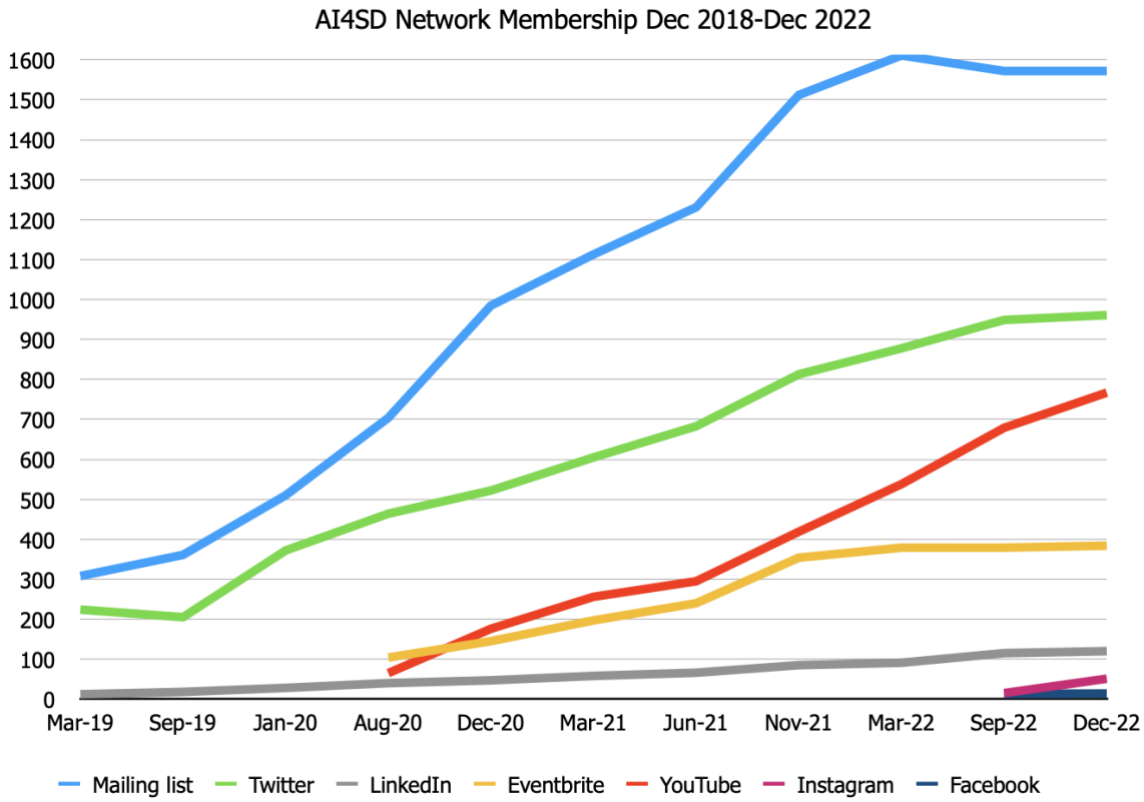


Figure 1: Network Membership Growth between December 2018 to December 2022

2.2.2. Events

Through the last four years the Network has run 65 events, starting with our launch event in December 2018. The events before COVID-19 were all ran as physical events, and we converted to running virtual events in summer 2022 when we started our first online seminar series. These were extremely popular, resulting in our network membership doubling and gaining an international presence since it greatly diversified who was able to attend these meetings. We returned with a hybrid conference in March 2022 and since have run a combination of hybrid and virtual events, noting that our members found this model substantially more inclusive. Table 3 denotes the different types of events that were run.

Table 3: Event Statistics

Type	Numbers	Type
Conference	4	2 Physical 1 Virtual 1 Hybrid
Workshops/Seminars	42	12 Physical 29 Virtual 1 Hybrid
Training Events	14	14 Virtual
Summer School	2	1 Physical 1 Hybrid
Hackathon	3	1 Physical 2 Hybrid

Our events drew a range of participants, there were a clear group of core Network Members who regularly attended events, but due to the popularity and diversity of the meeting topics each event brought new faces. Appendix E. Event Attendance contains a full list of our event attendance.

We had three big Network conferences throughout the last four years. First was our launch event in December 2018 to introduce the Network and the team. This launch featured seven speakers covering different aspects of AI and Machine Learning in healthcare, drug discovery, molecules and materials, in addition to discussing data and the philosophical aspects of AI. This event was held at the SCI in London and was attended by 104 people and served as an excellent introduction. A blog post about the event can be found on our website: https://www.ai4science.network/2018/12/05/05-12-2018-ai3sd-launch/ written by Michelle Pauli who also produced a formal report on the event: https://eprints.soton.ac.uk/427810/.

The second big conference was run in November 2019 to showcase our first year of activities and report on our funded projects. This conference ran over 2 days at the Winchester Holiday Inn, and featured some keynote industry speakers including Dr Andrew Senior from DeepMind to discuss Alphafold and Dr Richard Tomsett from IBM who talked about AI and Explainability. The conference also featured keynotes from academics working in highly relevant areas such as Dr Lucy Colwell from the University of Cambridge discussing protein prediction and Professor Juan Garrahan from the University of Nottingham discussing his work in non-equilibrium physics and machine learning methods. There was a wide range of additional presentations and a number of posters were also presented, demonstrating the wide range of work in the AI for Scientific Discovery area and showcasing the need for the Network to bring these communities together. A blog post about the event can be found on our website: https://www.ai4science.network/2019/11/18/ai3sd-conference-blog-post/ written by Michelle Pauli who also produced a formal report on the event: https://eprints.soton.ac.uk/444601/

Finally we ran a hybrid conference in March 2022 to round up the activities of the Network and talk about the future. This was a three day hybrid event at Chilworth Manor Hotel that opened with a retrospective from our PI Professor Jeremy Frey on our Network. The event featured a number of diverse sessions considering AI and ML in medicine, chemicals, molecules and materials, and talks on different techniques in these technologies, and other important aspects such as opacity, explainable AI and ethics. The event also featured three panel sessions which generated a lot of lively conversation, and presentations from a number of ECRs and PhD students who were funded by the Network either for pilot projects or internships. This conference was sponsored by Digital Discovery, CAS, Patterns, BSI and Dotmatics. A formal report was written on this event by Dr Wendy Warr and is available here: https://eprints.soton.ac.uk/471408/.

3. Outputs

This section details the different types of Outputs that were created as part of the Network activities, both with respect to outputs produced directly through events, funded projects and the journal and conference papers that were supported by the Network.

3.1. Event Outputs

Our events produced a range of outputs. For a majority of our events, including all conferences and workshops where material was presented around specific subjects, formal reports were written, either by members of the Network team where they had the appropriate expertise, or external members were brought in such as Michelle Pauli and Dr Wendy Warr to produce formal conference reports. Since COVID-19 and taking the Network activities online, we started producing videos for our YouTube Channel. Almost every talk given as part of our online/hybrid events (apart from where speakers did not give permission) has been captured and made available on our YouTube Channel. We also ran a number of interviews with speakers and funded project members, which were particularly useful during COVID-19 where members were missing some of the usual networking that would occur during events, and so could at least find out more about our speakers in relation to the Network. We also offered Network members the opportunity to present 44 posters across several of our events, enabling them to showcase their work to Network members. Table 4 contains the totals for these different outputs. All of these outputs have been deposited into our ePrints repository and have their own DOIs.

Table 4: Event Outputs for the Network

Type	Numbers
Event Reports	25
Videos	174
Speaker Interviews	39
Posters	44

When we started producing videos, we set up the AI4SD YouTube Channel which has gone from strength to strength. The top three videos and their views are detailed in Table 5 and the full list of videos are listed in A.2. Videos.

Table 5: Top 3 YouTube Videos

Video	Link	Views
Skills4Scientists – Intro to Python 1 – Using RDKit in Anaconda – *Mr Samuel Munday*	https://youtu.be/kg6puavKMz8	2700
AI3SD Summer Seminar Series 2: InChl: Measuring the Molecules – *Professor Jonathan Goodman*	https://youtu.be/B881b5BasnU	1547
AI4Proteins: General Effects of AI on Drug Discovery – *Dr Derek Lowe*	https://youtu.be/YJg0WwUANEQ	834

3.2. Funded & Publication Outputs

The Network also funded several different projects including pilot projects and internships, and all of these required a project report to be created. Additionally, some of our Machine Learning summer school students produced project reports to detail their hackathon efforts. The Network also supported several publications that were produced as a result of Network funded research. Table 6 contains the number of reports and publications that were produced

by the Network, and Appendix B. Funded Project Reports and Appendix C. Journal and Conference Papers contains a full list of all of these reports and publications with DOI links.

Table 6: Funded Project Reports & Journal/Conference Publications

Type	Numbers
Pilot Project Reports	7
Intern Project Reports	12
Summer School Project Reports	8
Journal & Conference Papers	19

3.3. AI4SD Attended Events

Some resources were also produced about AI4SD to showcase our Network to other communities, Table 7 summarises the posters and presentations created about AI4SD and there are further details in Appendix D. Presentations & Posters about AI4SD.

Table 7: Resources produced about AI4SD

Type	Number
Presentation	3
Posters	2

4. Funded Initiatives

Throughout the Network term, we funded 7 pilot projects, 15 interns and over 120 students across two machine learning summer schools. We asked the people we funded to provide an impact statement about how our funding helped them and surveyed the summer school students to understand their experiences. Overall, our funding seems to have had a very positive impact on those who received it and this section contains direct written statements from a number of these people.

4.1. Pilot Projects

Prof Matthew Todd – UCL – Funded as part of our first funding call.
The AI3SD funding allowed us to run a unique competition that led to the public demonstration of the effectiveness of AI and machine learning methods for drug discovery. Our consortium, Open-Source Malaria, hosted potency data on around 400 molecules in a particular antimalarial series. It was challenging to predict new molecules that would be potent. We invited companies (and anyone else) to submit models to us that would accurately predict potency for a test set that we kept out of public view. Those models scoring best were invited to submit new structures for us to synthesise and evaluate. We therefore completed the cycle of model generation, validation, prediction and evaluation. The new molecules made had a 50% success rate of activity vs the malaria parasite. The competition was highly unusual: since all data and ideas were publicly available in real time, the private sector took part despite the risk of losing. The winning team was able to use their performance to advertise their capabilities. Thus, an open science competition can help the private sector while progressing drug discovery against

a tropical disease. The work was published (10.1021/acs.jmedchem.1c00313). We have since continued to work with two organisations to refine the predictive models; one of these projects (with Ersilia.io) is supported by a small grant from the Rosetrees Trust. We have also secured proof of concept funding from a UCL-EPSRC funding pool for a related project in the area of generative methods in biomolecule prediction vs an antibacterial protein, the results from which will be available in October 2022 (https://github.com/opensourceantibiotics/murligase/issues/69). A larger-scale version of this idea, known as CACHE, is now running (10.1038/s41570-022-00363-z).

Prof Tim Albrecht – University of Birmingham – Funded as part of our first funding call.
The funding has had multiple impacts. It allowed us to explore new AI tools, for example Capsule Nets for event detection, which was part of the original funded project. In that context, we also found a new approach for feature detection in single-molecule data, based on Image Recognition/ Transfer Learning and dimensionality reduction. Two papers have been published:

- https://iopscience.iop.org/article/10.1088/2632-2153/aba6f2/meta
- https://pubs.rsc.org/en/content/articlehtml/2022/cc/d2cc03187f (as part of the Pioneering Investigator Themed Issue).

The meetings have been great platform to engage with others in the field and have inspired some very nice new work. Two of my students also took part in the summer school and contributed as tutors for a data challenge I set (around detecting anomalies). Continuous engagement with the community has also allowed me to progress research collaborations in this space, internally (with colleagues in Comp Sci at UoB, leading to joint UG and MSc projects) as well as elsewhere (e.g., with colleagues at the CitAI Research Centre at City, University of London; I am giving a talk there in December).

Dr Keith Butler – UCL (Formerly STFC) Funded as part of our second funding call
The AI3SD grant was a huge help for seeding my research programme in machine learning for analysis of tomography data. The grant allowed me to work closely with Finden an SME based at Harwell and together we developed a number of approaches that go beyond the state of the art in chemical tomography, including classifying regions of tomographs, improving reconstruction quality and removing noise from collected data. The work funded by AI3SD formed the basis of an on-going programme of work that has since been funded by an Innovate A4i grant and an STFC Cross-Cluster grant with the ISIS Neutron and Muon Source. We have also published a paper based on the work started with this grant (https://www.nature.com/articles/s41524-021-00542-4)* and the methods developed are being applied by Finden in analysis of real industrial tomography data.

Dr Paul Dingwall – Queens University Belfast – Funded as part of our second funding call
As an early career researcher, still on probation in 2020, receiving funding from AI3SD was close to career changing. Still at the start of my career, I am in the process of finding my feet and defining my own direction as a researcher. I am a physical organic chemist with expertise in the study of mechanisms in homogeneous catalysis using traditional kinetic, synthetic, and computational (DFT) techniques. I am hugely interested in the application of machine learning and data science to physical organic chemistry, particularly in finding a way to use kinetic data with these techniques. My eventual goal is to show that modern, data rich techniques can

allow us to gain insights into whole classes of reaction in a single study, as opposed to the more traditional one reaction at a time approach. However, I lacked the means with which to start any investigation.

The big problem with machine learning is the requirement for huge amounts of data. In existing uses of machine learning in chemistry, high throughput techniques have been used to collected single timepoint yield data (one sample after a set time) of several thousand reactions to feed an algorithm. Kinetic study (multiple samples over the course of a reaction) lacks high throughput methods and so is significantly more time consuming and will generally take as long as the reaction takes to reach completion. But kinetic data should be far more valuable than single timepoint yield data. We hypothesised that using kinetic data would allow prediction of the time taken for a reaction to reach completion while also providing insight on reaction mechanism across a whole class of reaction. Neither of these goals are currently possible with existing approaches to machine learning in chemistry. We also aim to apply a machine learning technique called active learning. This is a cutting-edge machine learning technique, not yet widespread even in the computer science literature, and should allow us to build better models using minimal data sets.

Receiving this funding allowed me to test these ideas and approaches by purchasing materials and hiring a PDRA to collect data in the lab, allowing 310 full kinetic profiles to be collected over 6 months of lab time. The result will be an eventual publication with which I aim to form the basis of a new line of future grant proposals to continue this research. Most importantly though, this funding has allowed me to build a collaboration with a colleague in Computer Science at QUB. There are very few instances, that I am aware of, of collaboration across Chemistry and Computer Science and this will hopefully herald the start of a long a fruitful partnership. AI3SD have also been fantastic in helping me raise my profile, with additional funding to visit conferences, receipt of a poster prize, a published interview, and an invitation to present my research at a future date.

Dr Grant Hill – University of Sheffield – Funded as part of our second funding call
The funding of our project has helped define new research directions for my group, all of which are associated with artificial intelligence and/or automated design in the physical sciences. The project itself was concerned with the design of new materials, but the skills and knowledge acquired during this project has been incorporated into other activities, which has led to a successful EPSRC proposal on machine learning basis sets in quantum chemistry (grant EP/T027134/1). The visibility afforded by the award and associated network activities, including invited conference talks, has enabled me to grow my personal network of researchers using AI for scientific discovery and has culminated in me leading a "Creating and using molecules and materials" interest group of the Sheffield AI network (affiliated with the Turing institute).

4.2. Internship Programmes

Professor Jonathan Hirst – University of Nottingham – Funded as part of our Internship Funding Call

The summer project studentship funded by the AI3SD network in 2021 allowed us to conduct some exploratory research into solvent selection for sustainable chemistry, which has subsequently formed a significant line of inquiry in our group. This is being taken forward by a postdoc and also involves a collaboration with a computer scientist at the University of Vienna. Some preliminary results will be presented as a poster at the RSC conference on "Artificial Intelligence in Chemistry" in September 2022. We anticipate a full peer-reviewed publication in due course. Ultimately, the software tool developed from the research will be integrated into our one-stop platform for sustainable chemistry, AI4Green, which, with funding from the Royal Academy of Engineering, is combining an Electronic Laboratory Notebook (ELN) with route prediction, reaction selectivity prediction, and Life Cycle Assessment.

Mr Samuel Munday – University of Southampton – Funded as part of our Internship Funding Call

The development of new and novel antimicrobial compounds is a costly and lengthy process with very little economic benefit for the pharmaceutical companies that develop them. With the rise of antimicrobial resistance globally, the majority of new antibiotics become antibiotics of last resort, shelved for the future making it very difficult for the creators to recoup the costs of development. Therefore, it falls to academic institutions to lead the research cycle of these compounds, often with far less budget and resource than their industrial counterparts. The work that is carried out is often experimentally led, with vast amounts of data being produced in silos and never leveraged at scale. Work is often repeated, data doesn't provide the value it should, the speed at which progress is made is limited and costs are higher as the chances of success are reduced.

Supramolecular self-associating amphiphiles (SSAs) are a class of amphiphilic salt which have demonstrated antimicrobial activity against both Gram-positive and Gram-negative bacteria. The Hiscock group run an international consortium of researchers who are studying the efficacy of SSA's experimentally. A small 12-week project was set up with AI4SD between UCL, University of Southampton and University of Kent to study the effectiveness of predictive modelling for the development of new and novel SSA molecules.

Machine learning offered an opportunity to leverage the vast amount of data that has been generated across the Hiscock consortia at scale. In doing so it has the potential to act as a method of screening thousands of experimental pathways, saving time and money by driving the direction of the work carried out in the lab. The opportunity to improve the chances of success were predicted to be vast by all parties involved including UKHSA.

This 12 week-long exploratory project, carried out by Kaley Patel, under the supervision of Jennifer Hiscock, Cally Haynes, and Samuel Munday looked into the feasibility of using machine learning to model a small set of the consortiums data. It was found that some work was needed to extract data from across the consortia, and some extra work needed to turn this data into a useful dataset, but that the application of random forest models on the cleaned data generated results that were similar to those seen experimentally. At the end of the 12

weeks, it was clear where the issues lay in collaborating across research groups and what the barriers were to implementing successful ML models. However, most importantly, the results were promising enough that we had validated the need for a much larger scale project.

The learnings and success of this exploratory work directly led to a much-expanded remit. It was clear that, modelling aside, the data the consortia generated needed to be centralised, with clear standards set for the recording and indexing of the scientific work. Only then could more sophisticated and powerful ML models be applied to further the groundwork that had been done by Kaylee. This was a much larger project that was given to a masters student in the Frey group, who has successfully implemented data standards, created a relational database and carried out advanced ML aiding the Hiscock consortia in their search for the next generation of antimicrobial compounds.

4.3. Summer Schools

We ran two Machine Learning Summer Schools, one virtually in Summer 2021 and one as a hybrid event in Summer 2022. Across these two schools we supported over 120 students to upskill them in different aspects of Machine Learning and other useful skills drawn from our Skills4Scientists series. We sent out feedback forms for both events to see how well they were received by our students

4.3.1. Machine Learning for Materials & Chemicals Summer School 2021

This summer school was run in conjunction with the Directed Assembly Network and was run virtually due to COVID-19. It was run across 8 weeks on Tuesday afternoons, and included a mixture of lectures, and group work finishing with group presentations on the final week. Each group was given a mentor to support their project.

Overall, most students said they were very satisfied with the summer school, but they gave us some useful feedback which we put into place for our second summer school. The students noted that they wanted the school to start with some more introductory sessions and raised a desire for some more hands on practical sessions with more interaction with their mentors. When we asked if they would want the school to run physically virtually or hybrid the year after they all voted for either in person or hybrid.

4.3.2. Machine Learning Summer School 2022

Taking the feedback on board from the previous year, we ran our 2022 summer school as a week-long hybrid course at the University of Southampton and on Zoom. We organised some introduction to python sessions at the beginning of day 1 with an example Jupyter Notebook as was requested in the previous feedback. As with the previous year we split the students into teams for a hackathon, we brought in helpers for the hackathon sessions so that the groups could have hands on help.

Again, the summer school was very well received overall. There was still feedback that some students would have liked more introductory material at the beginning, especially more python training. Next time we run one of these events we are considering either running multiple ones at different levels, or potentially assigning a full 2 days to hands on phyton training at the beginning.

We also asked students what other sorts of events they would like to see us run, and there was a clear appetite for more summer schools, events on Python and ML for chemical applications, more basic training courses, sessions on other coding languages such as R (which we subsequently addressed in one of our latest events).

5. Other Outputs

The Network also worked on a number of other projects with the Network of Networks and co-funded an Ethics for AI working group. This section describes these initatives.

5.1. Network of Networks

https://network-mgmt.ai3sd.org/

This resource has been produced by a group of diverse research management professionals, representing different disciplines and organisations to aid Network Managers and Investigators in the creation and management of research communities. They have drawn together their collective experience in managing different aspects of these NetworkPluses to produce advice and tips for best practices.

5.2. ED&I in AI4SD

ED&I is clearly an issue for every Network+. At AI4SD we have tried to address it, although it is very hard to track it in a non-invasive manner. As part of our work to address ED&I issues, we collaborated with the Network of Networks Group to run an ED&I Survey across 2021 and 2022 and have been using the results to influence how we run our Network. We have also run and taken part in ED&I workshops, in addition to running an ECR workshop with an ED&I discussion group.

The results of our ED&I survey were written up as part of a conference presentation: Chandler-Wilde, S., Kanza, S., Fisher, O., Fearnshaw, D. and Jones, E., 2022. Reflections on an EDI Survey of UK-Government-Funded Research Networks in the UK.

5.3. Ethics for AI group

AI4SD co-funded an interdisciplinary Ethics for AI Group with the Internet of Food Things Network, which comprises of 6 multidiscipline researchers at different universities. This group was set up to consider the ethical dimensions of digital collaboration in the food sector, such as the unintended consequences of AI. The groups aims were:

- To explore and support ethical challenges in developing food data trusts, particularly if they incorporate use of AI and related technology
- Using speculative methods to develop a framework of ethical evaluation
- To support ethical practice for data sharing in the food industry

This work was undertaken throughout 2020-2022 and has produced the following research papers (noted above). The group is now working on a large-scale proposal for EPSRC funding.

Appendices

Appendix A: Event Outputs

This section will detail all the different types of Event Outputs that were produced by the Network, including Event Reports, Videos, Q+As, Interviews and Posters.

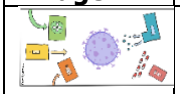
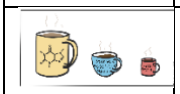
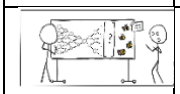
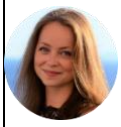
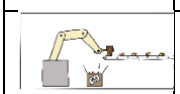
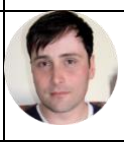
A.1. Event Series Reports

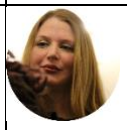
Report Details	Author
AI4SD-Event-Series:Report-1: Semantics 2018	Dr Samantha Kanza
AI4SD-Event-Series:Report-2: PhenoHarmonIS 2018	Dr Samantha Kanza
AI4SD-Event-Series:Report-3: Machine Intelligence Showcase 2018	Dr Samantha Kanza
AI4SD-Event-Series:Report-4: AI3SD Network+ Launch 2018	Michelle Pauli
AI4SD-Event-Series:Report-5: Recoding Black Mirror Workshop 2019	Dr Samantha Kanza
AI4SD-Event-Series:Report-6: Molecules, Graphs & AI Workshop 2019	Dr Nicola Knight
AI4SD-Event-Series:Report-7: AI in Drug Discovery & Drug Safety Workshop 2019	Dr Wendy Warr
AI4SD-Event-Series:Report-8: AI in Materials Discovery Workshop 2019	Dr Nicola Night & Dr Colin Bird
AI4SD-Event-Series:Report-9: Paperless Lab Conference 2019	Dr Samantha Kanza & Dr Nicola Knight
AI4SD-Event-Series:Report-10: Semantics & Knowledge Learning for Chemical Design Workshop 2019	Dr Samantha Kanza
AI4SD-Event-Series:Report-11: Machine Learning for Materials Science Workshop 2019	Dr James Cumby
AI4SD-Event-Series:Report-12: 10th Triennial Congress of the International Society for Theoretical Chemical Physics 2019	Dr Grant Hill
AI4SD-Event-Series:Report-13: AL & ML in Chemical Discovery & Development 2019	Dr Bao Nguyen
AI4SD-Event-Series:Report-14: AI3SD & IoFT AI for Allergen Detection Workshop Report 2019	Michelle Pauli
AI4SD-Event-Series:Report-15: AI3SD Network+ Conference Report 2019	Michelle Pauli
AI4SD-Event-Series:Report-16: AI3SD, OSM & RSC-CICAG Predicting the activity of Drug Candidates when there is not target Workshop Report	Dr Chris Swain
AI4SD-Event-Series:Report-17: AI3SD, Dial-a-Molecule & Directed Assembly: AIReact2020 Conference Report 2020	Dr Wendy Warr
AI4SD-Event-Series:Report-18: AI3SD AI4Good Workshop @ WebSci'20 Report 2020	Michelle Pauli
AI4SD-Event-Series:Report-19: Failed it to Nailed it! How to get data sharing right! – Dealing with Data: Tips & Tricks	Dr Samantha Kanza & Dr Nicola Knight
AI4SD-Event-Series:Report-20: Failed it to Nailed it! How to get data sharing right! – Data Standards	Dr Samantha Kanza & Dr Nicola Knight
AI4SD-Event-Series:Report-21: Failed it to Nailed it! How to get data sharing right! – Responsible Data Management	Dr Samantha Kanza & Dr Nicola Knight
AI4SD-Event-Series:Report-22: Failed it to Nailed it! How to get data sharing right! – Data Citations and Publishing	Dr Samantha Kanza & Dr Nicola Knight
AI4SD-Event-Series:Report-23: AI4Proteins: Protein Structure Prediction	Dr Wendy Warr
AI4SD-Event-Series: Report-24: AI4SD Conference	Dr Wendy Warr

A.2. Videos

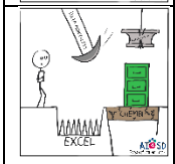
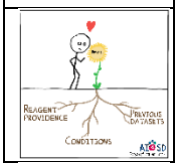
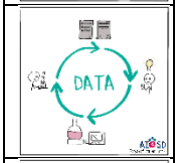
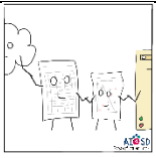
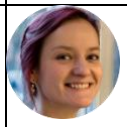
This section will detail all the different types of videos that were produced as part of the Network, organised by series.

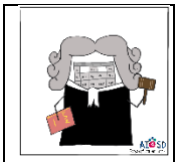
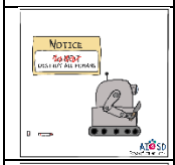
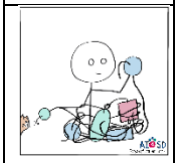
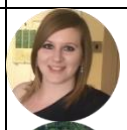
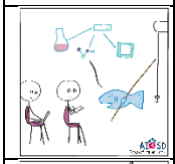
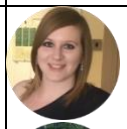
A.2.1 Summer Seminar Series

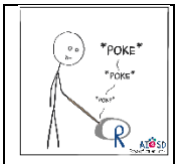
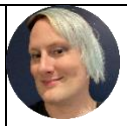
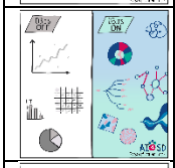
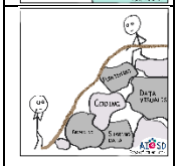
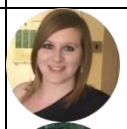
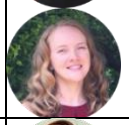
Image	Title	Video Link	DOI Link	Speaker
	Drug Repositioning for COVID-19	https://youtu.be/qcgeTVfiVl4	http://dx.doi.org/10.5258/SOTON/P0046	 Prof John Overington *Medicines Discovery Catapult*
	InChi: Mearsuring the molecules	https://youtu.be/B881b5BasnU	https://doi.org/10.5258/SOTON/P0047	 Prof Jonathan Goodman *University of Cambridge*
	Design Fiction as a Method, and why we might use it to consider AI	https://youtu.be/AxXZRk6CLws	http://dx.doi.org/10.5258/SOTON/P0048	 Dr Naomi Jacobs *University of Lancaster*
	Neural Networks and Explanatory Opacity	https://youtu.be/3rSnjnUjpo0	http://dx.doi.org/10.5258/SOTON/P0049	 Dr Will McNeill *University of Southampton*
	Dimensionality in Chemistry: Using Multidimensional data for Machine Learning	https://youtu.be/NhR7xWlAO4g	http://dx.doi.org/10.5258/SOTON/P0050	 Dr Ella Gale *University of Bristol*
	Quantum Computing: A Guide for the Perplexed	N/A	N/A	 Prof Andy Stanford-Clark *IBM*
	Artificial Intelligence's new clothes? From General Purpose Technology to Large Technical System	https://youtu.be/WyB42XTI4VA	http://dx.doi.org/10.5258/SOTON/P0051	 Dr Simone Vannuccini *University of Sussex* &  Ms Ekaterina Prytkova *Friedrich Schiller University Jena*
	Smart cleaning & COVID-19	https://youtu.be/o3TSkGgHI78	http://dx.doi.org/10.5258/SOTON/P0057	 Dr Nicholas Watson *University of Nottingham*
	The Bluffers Guide to Symbolic AI	https://youtu.be/Gc7MGnQ4mEk	http://dx.doi.org/10.5258/SOTON/P0058	 Dr Louise Dennis *University of Manchester*
	Machine Learning for Early Stage Drug Discovery	https://youtu.be/GY0myVuhrCo	http://dx.doi.org/10.5258/SOTON/P0056	 Prof Charlotte Deane *University of Oxford*
	Using Artificial Intelligence to Optimise Small-Molecule Drug Design	N/A	N/A	 Dr Nathan Brown *Benevolent AI*

	On the Basis of the Brain: Neural-Network-Inspired Changes in General Purpose Chips	https://youtu.be/tza5n1XiEGg	http://dx.doi.org/10.5258/SOTON/P0055	 Dr Simone Vannuccini *University of Sussex* &  Ms Ekaterina Prytkova *Friedrich Schiller University Jena*
	Supramolecular antimicrobials – the next target for AI/Machine Learning	https://youtu.be/fWR1Ox19wws	http://dx.doi.org/10.5258/SOTON/P0054	 Dr Jennifer Hiscock *University of Kent*
	AI for Science: Transforming Scientific Research	https://youtu.be/qptQG5o0HN0	http://dx.doi.org/10.5258/SOTON/P0053	 Prof Tony Hey *STFC*

A.2.2. Data Seminar Series

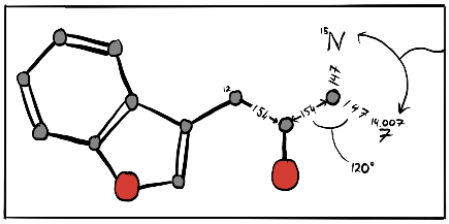
Image	Title	Video Link	DOI Link	Speaker
	Love notes to the future: the importance of metadata	https://youtu.be/bvD7k5xKnXo	http://dx.doi.org/10.5258/SOTON/P0032	 Isobel Stark *University of Southampton*
	Pitfalls and Gotcha's with bioactivity data	https://youtu.be/EoZfoQlAKqo	http://dx.doi.org/10.5258/SOTON/P0032	 Prof John Overington – Medicines Discovery Catapult
	Digitising your Chemistry for Recordability, Shareability and Reproducibility	https://youtu.be/BLf-M4xWITM	http://dx.doi.org/10.5258/SOTON/P0069	 Dr Mark Warne *Deep Matter*
	Data Generation, Data Standards and Metadata Capture in Drug Discovery	https://youtu.be/t3R6BV_8XGI	http://dx.doi.org/10.5258/SOTON/P0064	 Dr Martin-Immanuel Bittner *Arctoris*
	Giving your Open Data the best chance to realise its potential	https://youtu.be/3SvkOjEOCqc	http://dx.doi.org/10.5258/SOTON/P0065	 Mr Chris Gutteridge *University of Southampton*
	Linked Data – Examples and Heuristics	https://youtu.be/Q8l8Y-44fqo	http://dx.doi.org/10.5258/SOTON/P0066	 Dr Terhi Nurmikko-Fuller *Australian National University*
	Ethical data management – balancing individual privacy and public benefit	https://youtu.be/J9kWkzK83i4	http://dx.doi.org/10.5258/SOTON/P0059	 Zosia Beckles *University of Bristol*

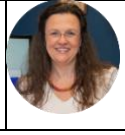
	Data legislation, personal and non-personal data, ethical issues and protecting your IP right	https://youtu.be/w5v5d6r6irs	http://dx.doi.org/10.5258/SOTON/P0060	 Michele Voznick *Pinsent Masons LLP*
	Practical Ethics for Data Science and Algorithm Design	https://youtu.be/jEFu1ykVI_I	http://dx.doi.org/10.5258/SOTON/P0061	 Tessa Darbyshire *CellPress Patterns*
	Data publication – a personal tale	https://youtu.be/6SneQbYHwO0	http://dx.doi.org/10.5258/SOTON/P0062	 Dr Sarah Callaghan *CellPress Patterns*
	Publishing and citing data in practice	https://youtu.be/PpMOkTnBMlI	http://dx.doi.org/10.5258/SOTON/P0063	 Mr Jez Cope *British Library*
	The (long) journey from supporting information to Publishing and Finding FAIR data in chemistry	https://doi.org/10.14469/hpc/7629	https://doi.org/10.14469/hpc/7629	 Prof Henry Rzepa – Imperial College London
	Organising your Networks & Projects	https://youtu.be/oa_HhvOqY7Q	http://dx.doi.org/10.5258/SOTON/AI3SD0218	 Dr Samantha Kanza & Dr Nicola Knight *University of Southampton*
	Hints and tips for optimising your researchfish data	https://youtu.be/blGysUkVMcc	http://dx.doi.org/10.5258/SOTON/AI3SD0220	 Gavin Reddick *ResearchFish Limited*
	Capturing and Tracking your outputs	https://youtu.be/0R9lU632JCc	http://dx.doi.org/10.5258/SOTON/AI3SD0220	 Dr Samantha Kanza & Dr Nicola Knight *University of Southampton*
	Using Scopus and SciVal to track your research impact and find collaborators	https://youtu.be/wsYpdqQnb5o	http://dx.doi.org/10.5258/SOTON/AI3SD0221	 Christopher James *Elsevier*
	Introduction to Data Visualisation	https://youtu.be/Q_ngUSQQEJc	http://dx.doi.org/10.5258/SOTON/AI3SD0252	 Dr Rita Borgo *Kings College London*

	(Reproducible) Data Visualisation with R and how to make interactive things with R	https://youtu.be/rnwYHJDgEHA	https://doi.org/10.5258/SOTON/AI3SD0253	 Miss Charlie Hadley *Visible Data Ltd*
	Data Visualisation with Python	https://youtu.be/Atr2-34r2GM	https://doi.org/10.5258/SOTON/AI3SD0254	 Mr Samuel Munday *University of Southampton*
	Visualize Your Data for the Web using D3.js	Not available	Not available	 Dr Alfie Abdul-Rahman *Kings College London*
	Introduction to Challenges	Not available	Not available	  Dr Samantha Kanza & Dr Nicola Knight *University of Southampton*
	Data Visualisation in Publishing & Communication	https://youtu.be/SkV491A8qgU	https://doi.org/10.5258/SOTON/AI3SD0255	 Dr Sarah Callaghan *CellPress Patterns*

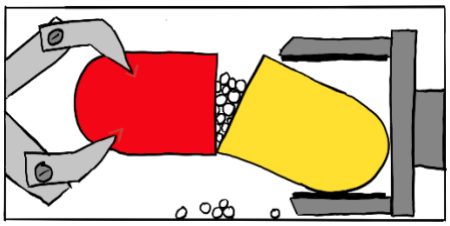
A.2.3. Winter Seminar Series 2020-2021

1. Topology & Applications in Chemistry



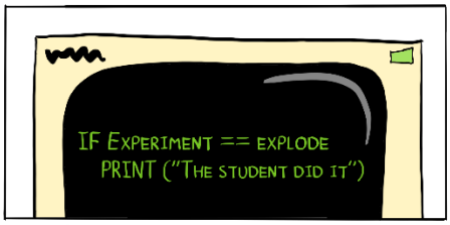
Talk	Video Link	DOI Link	Speaker
Topology: From Shapes to numbers	https://youtu.be/hbiuV1cH0gs	http://dx.doi.org/10.5258/SOTON/P0089	 Professor Jacek Brodzki *University of Southampton*
New theoretical and data-driven approaches to the study of molecular conformational spaces and energy landscapes	https://youtu.be/e7juNuMkvV0	http://dx.doi.org/10.5258/SOTON/P0088	 Dr Ingrid Membrillo Solis *University of Southampton*
The Shape of Data in Chemistry – Insights Gleaned from Complex Solutions and Their Interfaces	https://youtu.be/L51LHDHtoH4	http://dx.doi.org/10.5258/SOTON/P0087	 Professor Aurora Clark *Washington State University*

2. Robots, AI & NLP in Drug Discovery



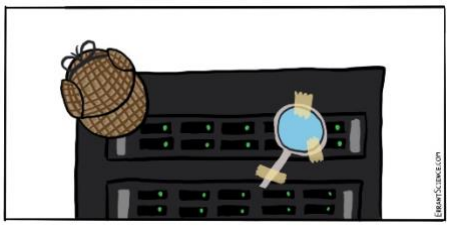
Talk	Video Link	DOI Link	Speaker
Natural Language Processing in AI-driven Drug Discovery: What it is, why it matters and how (not) to do it	N/A	N/A	 Dr Sia Togia *Benevolent AI*
New Trends in Drug Discovery	https://youtu.be/nWmZjcdxSp0	http://dx.doi.org/10.5258/SOTON/P0086	 Dr Martin-Immanuel Bittner *Arctoris*
An Open Competition of People and Machines to Develop Predictive Models for Antimalarial Drug Discovery	https://youtu.be/EpMEUU-K6Yk	http://dx.doi.org/10.5258/SOTON/P0085	 Prof Matthew Todd *University College London*

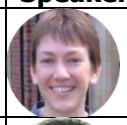
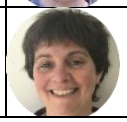
3. Enhancing Experiments through Machine Learning



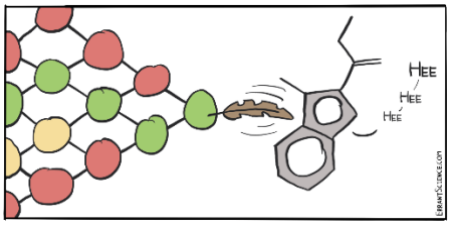
Talk	Video Link	Link	Speaker
Interpretable machine learning for materials design and characterization	https://youtu.be/pI-wCuj07oI	http://dx.doi.org/10.5258/SOTON/P0084	 Dr Keith Butler *STFC*
When charge transport data are a worn – a transfer learning approach for unsupervised data classification	https://youtu.be/Lma1qQ-B2Qo	http://dx.doi.org/10.5258/SOTON/P0083	 Prof Tim Albrecht *University of Birmingham*
Prediction in organometallic catalysis – a challenge for computational chemistry	https://youtu.be/4nvkh-nhaEc	http://dx.doi.org/10.5258/SOTON/P0093	 Dr Natalie Fey *University of Bristol*

4. ML 4 Scientific Discovery



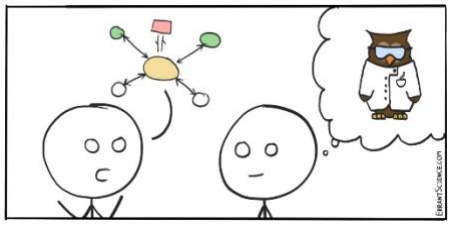
Talk	Video Link	DOI Link	Speaker
Data-driven materials discovery for functional applications	https://youtu.be/96_MY0nug3M	http://dx.doi.org/10.5258/SOTON/P0082	 Prof Jacqui Cole *University of Cambridge*
Outlier detection in Scientific Discovery	https://youtu.be/_bI948j46Ho	http://dx.doi.org/10.5258/SOTON/P0081	 Dr Jo Grundy *University of Southampton*

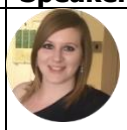
5. Graphs, Networks & Molecules



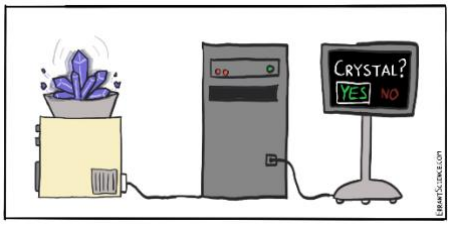
Talk	Video Link	DOI Link	Speaker
Machine Learning for electronically excited states of molecules	https://youtu.be/MqofIHXDVEo	http://dx.doi.org/10.5258/SOTON/P0080	 Dr Julia Westermayr *University of Warwick*
Machines Learning Chemistry	https://youtu.be/epdG4n-uTc	http://dx.doi.org/10.5258/SOTON/P0092	 Prof Jonathan Hirst *University of Nottingham*
Preserving Structural Motifs in Machine-Learning Approaches to Modeling Water Clusters	https://youtu.be/Dd2RbLFiSuU	http://dx.doi.org/10.5258/SOTON/P0079	 Dr Jenna A. Bilbrey – Pacific Northwest National Laboratories

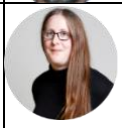
6. Semantic Web Technologies in Chemistry



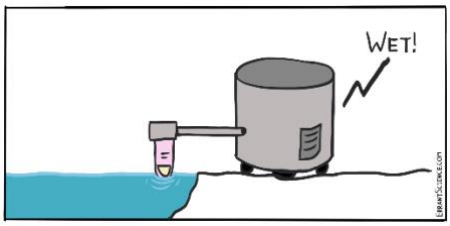
Talk	Video Link	DOI Link	Speaker
Semantic Web in Scientific Research – Possibilities & Practices	https://youtu.be/PmIwT-d05jU	http://dx.doi.org/10.5258/SOTON/P0078	 Dr Samantha Kanza *University of Southampton*
Ontologies, Natural Language, Annotation and Chemistry	https://youtu.be/Bl-8V48hjgc	http://dx.doi.org/10.5258/SOTON/P0077	 Dr Colin Batchelor *Royal Society of Chemistry*
H2020 Project Onto Trans	https://youtu.be/cBWwl-rgmyo	http://dx.doi.org/10.5258/SOTON/P0076	 Dr Alexandra Simperler *Goldbeck Consulting*

7. Materials Machine Learning



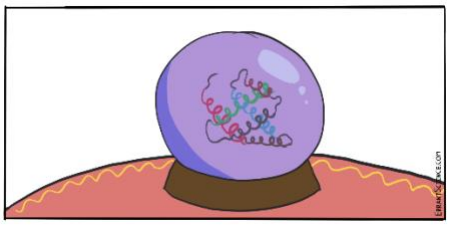
Talk	Video Link	DOI Link	Speaker
Deep Learning Enhanced Quantum Chemistry: Pushing the limits of Materials Discovery	https://youtu.be/wqN_BCU8514	http://dx.doi.org/10.5258/SOTON/P0075	 Dr Reinhard Maurer *University of Warwick*
Accelerating structure prediction models for materials discovery	https://youtu.be/FuWtSkfkxFI	http://dx.doi.org/10.5258/SOTON/P0074	 Prof Graeme Day *University of Southampton*
High-Throughput Approaches for the Discovery of Supramolecular Organic Materials: Fusing Computational Screening with Automated Synthesis'?	N/A	N/A	 Dr Becky Greenway *Imperial College London*

8. Property Prediction



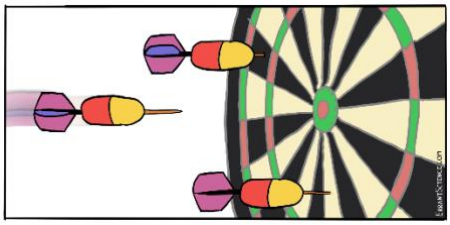
Talk	Video Link	DOI Link	Speaker
Generating a Machine-Learned Equation of State for Fluid Properties	https://youtu.be/mnVj8aM2xho	http://dx.doi.org/10.5258/SOTON/P0073	 Prof Erich Müller *Imperial College London*
Machine Learning with Causality: Solubility Prediction in Organic Solvents and Water	https://youtu.be/bDvJCFlQRcU	http://dx.doi.org/10.5258/SOTON/P0072	 Dr Bao Nguyen *University of Leeds*

9. AI 4 Proteins



Talk	Video Link	DOI Link	Speaker
Machine learning for biological sequence design	https://youtu.be/_LNsLNnEx7E	http://dx.doi.org/10.5258/SOTON/P0090	 Dr Lucy Colwell *University of Cambridge*
Machine learning applications for macro-molecular X-ray crystallography at Diamond	https://youtu.be/3cRclaxOHWE	http://dx.doi.org/10.5258/SOTON/P0091	 Dr Melanie Vollmar *Diamond*

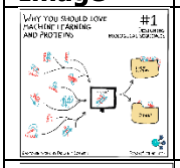
10. Targets



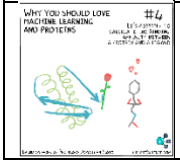
Talk	Video Link	DOI Link	Speaker
Using convolutional neural networks to enable neoantigen load as a biomarker of cancer immunotherapy	N/A	N/A	 Dr Felicia Ng *AstraZeneca*
Can Lattice Theory Help Find a Cure for Paralysis?	N/A	N/A	 Dr Nicola Richmond *GlaxoSmithKline*

A.2.4. AI 4 Proteins Seminar Series 2021

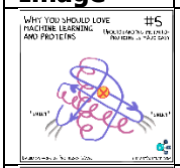
1. AI4 Proteins: I

Image	Talk	Video Link	Link	Speaker
	Machine learning for biological sequence design	https://youtu.be/_LNsLNnEx7E	http://dx.doi.org/10.5258/SOTON/P0090	 Dr Lucy Colwell *University of Cambridge*
	Machine learning applications for macro-molecular X-ray crystallography at Diamond	https://youtu.be/3cRclaxOHWE	http://dx.doi.org/10.5258/SOTON/P0091	 Dr Melanie Vollmar *Diamond*

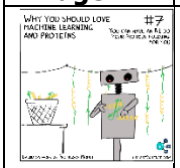
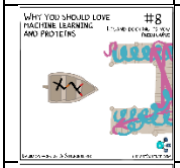
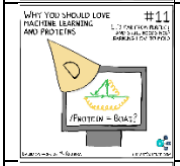
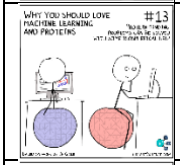
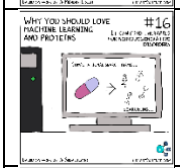
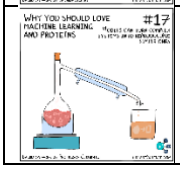
2. AI4 Proteins: II

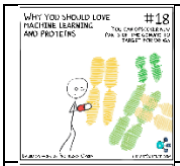
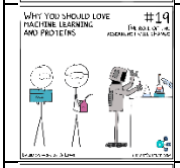
Image	Talk	Video Link	DOI Link	Speaker
	The Application of Machine Learning in Molecular Spectroscopy Study	https://doi.org/10.5258/SOTON/P0094	https://doi.org/10.5258/SOTON/P0094	 Prof Jun Jiang *University of Science and Technology China*
	Molecular Dynamics Simulations of Proteins	N/A	N/A	 Prof Jonathan Essex *University of Southampton*

3. AI4 Proteins: III

Image	Talk	Video Link	Link	Speaker
	Predicting Metalloproteomes by Machine Learning		N/A	 Prof Chu Wang *Peking University*
	Multiscale simulation of biomolecular mechanisms and dynamics: from enzyme evolution to receptor activation	https://youtu.be/wqP5tOmxAQs	http://dx.doi.org/10.5258/SOTON/P0127	 Prof Adrian J Mulholland *University of Bristol*

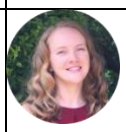
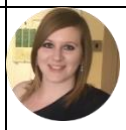
4. AI4 Proteins: Protein Structure Prediction

Image	Talk	Video Link	Link	Speaker
	An AI solution to the protein folding problem: what is it, how did it happen, and some implications	N/A	N/A	 Prof John Moult *University of Maryland*
	So you predicted a protein structure – What now?	https://youtu.be/e5ahKMf-inE	http://dx.doi.org/10.5258/SOTON/P0108	 Dr Thomas Steinbrecher *Schrödinger*
	Deep Learning enhanced prediction of protein structure and dynamics	https://youtu.be/E7eGHVybCH4	http://dx.doi.org/10.5258/SOTON/P0099	 Dr Martina Audagnotto *AstraZeneca*
	Fireflies-Lévy algorithm for peptides conformational optimization	https://youtu.be/DWNjqmCaUQc	http://dx.doi.org/10.5258/SOTON/P0109	 Dr Zied Hosni *University of Sheffield*
	How good are protein structure prediction methods at predicting folding pathways	https://youtu.be/XBz9KZMDApE	http://dx.doi.org/10.5258/SOTON/P0110	 Mr Carlos Outeiral Rubiera *University of Oxford*
	Protein-Ligand Structure Prediction for GPCR Drug Design	https://youtu.be/m8jwVmD4THq	http://dx.doi.org/10.5258/SOTON/P0112	 Dr Chris De Graaf *Sosei Heptares*
	Using icospherical input data in machine learning on the protein-binding problem	https://youtu.be/qAZtfhEZe9c	http://dx.doi.org/10.5258/SOTON/P0100	 Dr Ella Gale *University of Bristol*
	Lessons learned from generative models of biological sequences	https://youtu.be/3UeOFhsfFc8	http://dx.doi.org/10.5258/SOTON/P0101	 Prof Aleksej Zelezniak *Chalmers University of Technology*
	DeepDock: a deep learning approach to predict ligand binding conformations	https://youtu.be/j4qV6aew9cs	http://dx.doi.org/10.5258/SOTON/P0102	 Dr Oscar Mendez-Lucio *Janssen Pharmaceuticals*
	Finding new in silico-based therapeutic strategies for IAHSP	https://youtu.be/ciR0bXvyIoE	http://dx.doi.org/10.5258/SOTON/P0103	 Dr Matteo Rossi Sebastiano *University of Turin*
	Designing molecular models by machine learning and experimental data	https://youtu.be/DWbJS4bQ3uQ	http://dx.doi.org/10.5258/SOTON/P0104	 Prof Cecilia Clementi *Freie Universität*

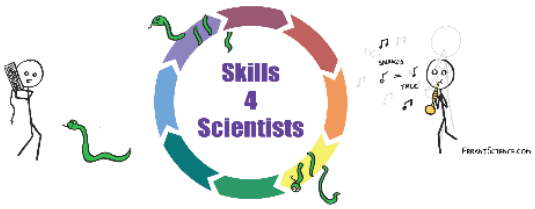
	The "almost druggable" genome	https://youtu.be/PezsuWDpvuI	http://dx.doi.org/10.5258/SOTON/P0105	 Prof Tudor Oprea *University of New Mexico*
	General Effects of AI on Drug Discovery	https://youtu.be/YJg0WwUANEQ	http://dx.doi.org/10.5258/SOTON/P0106	 Dr Derek Lowe *Novartis*
	Open Access Data: A Cornerstone for Artificial Intelligence Approaches to Protein Structure Prediction	https://youtu.be/73vXoH1vHG4	http://dx.doi.org/10.5258/SOTON/P0107	 Prof Stephen Burley *RCSB PDB, Rutgers University, UCSD*

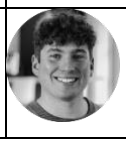
A.2.5. Skills 4 Scientists Seminar Series 2021

1. Research Data Management

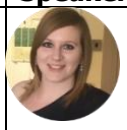
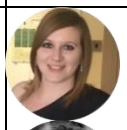
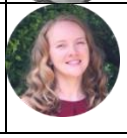
Title	Video Link	Link	Speaker
All's Fair in love and data management	https://youtu.be/NQ5pC1XoAHQ	http://dx.doi.org/10.5258/SOTON/P0113	 Ms Isobel Stark *University of Southampton*
Referencing and using Reference Managers	https://youtu.be/TrxGzlGom3o	http://dx.doi.org/10.5258/SOTON/P0114	 Dr Nicola Knight *University of Southampton*
Collaborative Data Management	https://youtu.be/a5kIcliML0Y	http://dx.doi.org/10.5258/SOTON/P0115	 Dr Samantha Kanza *University of Southampton*

2. Intro to Python 1

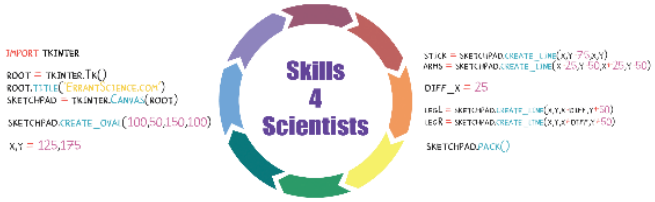


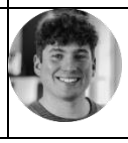
Title	Video Link	Link	Speaker
Setup, environments, installing packages, intro to Jupyter	https://youtu.be/qz7sVbDtnZc	http://dx.doi.org/10.5258/SOTON/P0116	 Mr Samuel Munday *University of Southampton*
Using RDKit	https://youtu.be/kg6puavKMz8	http://dx.doi.org/10.5258/SOTON/P0117	 Mr Samuel Munday *University of Southampton*

3. Version Control & LaTeX

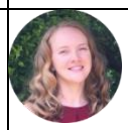
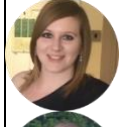
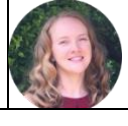
Title	Video Link	Link	Speaker
Introduction to LaTeX	https://youtu.be/z3Pu7LY4qr8	http://dx.doi.org/10.5258/SOTON/P0120	 Dr Samantha Kanza *University of Southampton*
Introduction to GitHub	https://youtu.be/Wfftr_d--28	http://dx.doi.org/10.5258/SOTON/P0121	 Mr Samuel Munday *University of Southampton*
Practical GitHub & Overleaf Demonstration	https://youtu.be/Ud24vdpd8Cs	http://dx.doi.org/10.5258/SOTON/P0122	  Dr Samantha Kanza & Mr Samuel Munday *University of Southampton*
Overleaf & LaTeX	https://youtu.be/8bnYwfWd3iw	http://dx.doi.org/10.5258/SOTON/P0123	 Dr Nicola Knight *University of Southampton*

4. Intro to Python 2

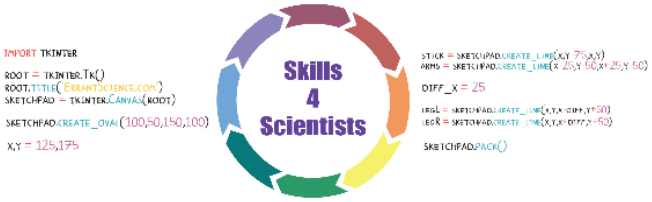


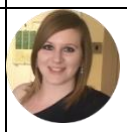
Title	Video Link	Link	Speaker
How to write good code	https://youtu.be/hxuUdpPMn1w	http://dx.doi.org/10.5258/SOTON/P0124	 Mr Samuel Munday *University of Southampton*
Typing, Variables, Data Types, Functions	https://youtu.be/tDKr6yE17ZY	http://dx.doi.org/10.5258/SOTON/P0125	 Mr Samuel Munday *University of Southampton*
Data Analysis Case Study	https://youtu.be/mUM4A9WKidc	http://dx.doi.org/10.5258/SOTON/P0126	 Mr Samuel Munday *University of Southampton*

5. Posters, Presentations & Reports

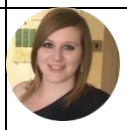
Title	Video Link	Link	Speaker
Writing a good Abstract & Best Practices for Scientific Communication	https://youtu.be/QIIkxhUHUSw	http://dx.doi.org/10.5258/SOTON/P0124	 Dr Sarah Callaghan *CellPress Patterns*
Presenting in Person & Online	https://youtu.be/ac5Tjv7pJHU	http://dx.doi.org/10.5258/SOTON/P0125	 Dr Nicola Knight – *University of Southampton*
Producing a good Poster		http://dx.doi.org/10.5258/SOTON/P0126	  Jonathan Lightfoot & Heather MacKenzie *University of Southampton*
Collaborative Reports/Presentations		http://dx.doi.org/10.5258/SOTON/P0139	  Dr Samantha Kanza & Dr Nicola Knight – *University of Southampton*

6. Careers 1



Title	Video Link	Link	Speaker
Writing a CV	https://youtu.be/9DdEwqqeB6A	http://dx.doi.org/10.5258/SOTON/P0140	 Dr Sarah Hewitt *University of Southampton*
Cultivating your Web Presence	https://youtu.be/D_auOMswtxk	http://dx.doi.org/10.5258/SOTON/P0141	 Dr Samantha Kanza *University of Southampton*
Building your professional contacts – Networking for Scientists and/or Introverts	https://youtu.be/Df2wrG_kDEA	http://dx.doi.org/10.5258/SOTON/P0146	 Dr Kevin Parker *KKI Associates*

7. Ethical Research

Title	Video Link	Link	Speaker
Intro to ethics	https://youtu.be/14nA9YBzBiI	http://dx.doi.org/10.5258/SOTON/P0147	 Dr Peter Craigon *University of Nottingham*
Writing an ethics application	https://youtu.be/sziOamD1k-Q	http://dx.doi.org/10.5258/SOTON/P0148	 Dr Samantha Kanza *University of Southampton*

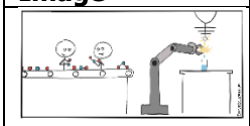
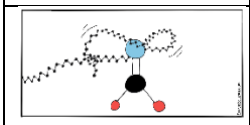
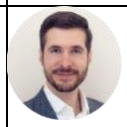
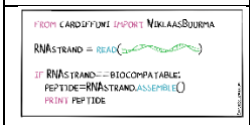
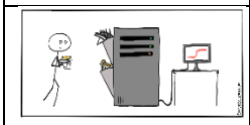
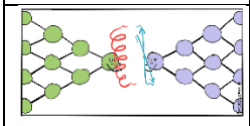
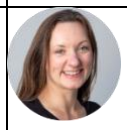
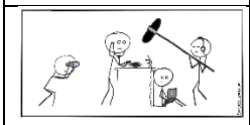
8. Careers 2

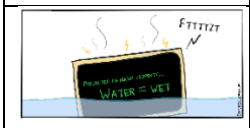
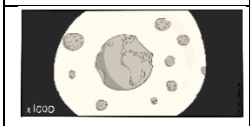
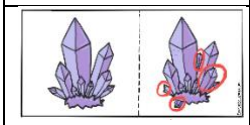
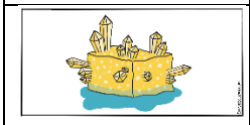
Title	Video Link	Link	Speaker
A career in Chemistry & Beyond	https://youtu.be/Df2wrG_kDEA	http://dx.doi.org/10.5258/SOTON/P0152	 Dr Kevin Parker *KKI Associates*

9. Posters & Career Symposium

Title	Video Link	Link	Speaker
Why you should take up PhD Opportunities in the Physical Sciences	https://youtu.be/f7pck610zyA	http://dx.doi.org/10.5258/SOTON/P0157	 Prof Jeremy Frey *University of Southampton*
Poster Compilation	https://youtu.be/vLVHqXyXlpA	http://dx.doi.org/10.5258/SOTON/P0158	Andras Vekassy; Anna Catton; Erhan Gulsen; Hewan Zewdu; Jamie Longio; Hongyang Dong; Kevin Daniel Calvache; Kaylee Patel; Aspen Fenzl; King Wong; Louis Greenhalgh; Maximillian Hoffmann; Rebecca Clements; Rubaiyat Khonder; Rhyan Barrett Thomas Allam; Sarah Scripps; Gavin Mann

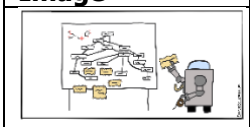
A.2.6. Machine Learning for Materials & Chemicals Seminar Series 2021

Image	Title	Video Link	Link	Speaker
	Directed Assembly of Materials – a 50 year retrospective	https://youtu.be/4ram0TaAVHU	http://dx.doi.org/10.5258/SOTON/P0128	 Prof Chick Wilson *University of Bath*
	Accelerated discovery for carbon capture solvents at IBM research	N/A	N/A	 Dr Flaviu Cipcigan *IBM*
	DNA: coding blocks for biocompatible assembly & disassembly	https://youtu.be/Ya38aMOFpOM	http://dx.doi.org/10.5258/SOTON/P0129	 Dr Niek Buurma *Cardiff University*
	Applying Machine Learning to Structured Time-course sensor data for Improved Chemical Outcomes and Reproducibility	https://youtu.be/FBJ3ZpBI5u8	http://dx.doi.org/10.5258/SOTON/P0130	 Dr David Pattison *Deep Matter*
	Assembling peptide and protein structures	https://youtu.be/md_VXdBLhpo	http://dx.doi.org/10.5258/SOTON/P0131	 Dr Anna Peacock *University of Birmingham*
	How to detect unexpected features and physical processes in single-molecule data	https://youtu.be/g2KNWfGkDDM	http://dx.doi.org/10.5258/SOTON/P0132	 Dr Tim Albrecht *University of Birmingham*
	Machine Learning with Causality in Chemistry	https://youtu.be/rF4CVXNLMkU	http://dx.doi.org/10.5258/SOTON/P0133	 Dr Bao Nguyen *University of Leeds*

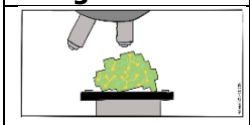
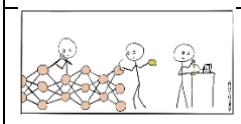
	Light and Directed Assembly	N/A	N/A	 Prof Julia Weinstein *University of Sheffield*
	Calibrated deep representations and entropy based active learning for materials property prediction	https://youtu.be/y_CvU01P0SU	http://dx.doi.org/10.5258/SOTON/P0143	 Dr Keith Butler *STFC*
	The Vast World of Very Small Holes: Metal-Organic Frameworks and Microporus Materials	N/A	N/A	 Dr Timothy Easun *Cardiff University*
	Quantifying crystal similarity to predict material properties	https://youtu.be/Pj3yUd1BVRU	http://dx.doi.org/10.5258/SOTON/P0142	 Dr James Cumby *University of Edinburgh*
	Simulation of chemical dynamics and spectroscopy with deep learning representations of electronic structure	https://youtu.be/IMJkcNtQgDo	http://dx.doi.org/10.5258/SOTON/P0145	 Dr Reinhard Maurer *University of Warwick*
	Using machine learning for discovery in supramolecular materials	N/A	N/A	 Dr Kim Jelfs *Imperial College London*
	Understanding the solid form: Structural Systematics Crystal Sponges	https://youtu.be/T4LYcmTVDnQ	http://dx.doi.org/10.5258/SOTON/P0144	 Prof Simon Coles *University of Southampton*

A.2.7. Autumn Seminar Series 2021

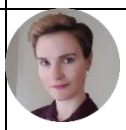
1. AI4SD Autumn Seminar I: Linked Data, Ontologies & Deep Learning

Image	Talk	Video Link	Link	Speaker
	Automated Chemical Oncology Expansion	https://youtu.be/dqYzFqw_SIU	http://dx.doi.org/10.5258/SOTON/AI3SD0154	 Dr Janna Hastings *Otto-von-Guericke University & UCL*
	Towards Biological Plausibility Using Linked Open Data	https://youtu.be/UN1YZBaciMM	http://dx.doi.org/10.5258/SOTON/AI3SD0155	 Dr Egon Willghagen *Masstricht University*

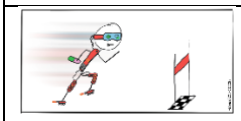
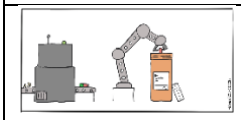
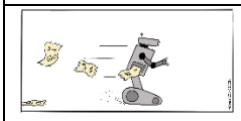
2. AI4SD Autumn Seminar II: Explainable AI & ML

Image	Talk	Video Link	Link	Speaker
	How can Explainable AI help scientific exploration	https://youtu.be/uokmY3cVdWw	http://dx.doi.org/10.5258/SOTON/AI3SD0156	 Prof Carlos Zednik *Eindhoven University of Technology*
	Explainable Machine Learning for Trustworth	https://youtu.be/IdOvoYAf2Kg	http://dx.doi.org/10.5258/SOTON/AI3SD0157	 Dr Fosca Giannotti *University of Pisa*

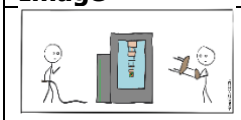
3. AI4SD Autumn Seminar III: Data Science 4 Chemistry

Image	Talk	Video Link	DOI Link	Speaker
	Statistics Are a Girl's Best friend: Expanding the mechanistic Study Toolbox with Data Science	https://youtu.be/c41ibgeX3Xw	http://dx.doi.org/10.5258/SOTON/AI3SD0158	 Dr Anat Milo *Ben-Gurion University of Negev*
	Data management: at the root of high-throughput experimentation	https://youtu.be/yXXm351nhjo	http://dx.doi.org/10.5258/SOTON/AI3SD0159	 Dr Nessa Carson *Syngenta*

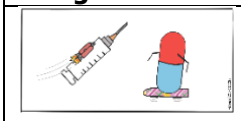
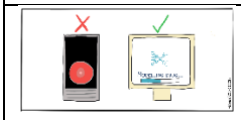
4. AI4SD Autumn Seminar IV: AI & ML 4 Drugs & Materials

Image	Talk	Video Link	Link	Speaker
	Combining robotics and Machine Learning for accelerated drug discovery	https://youtu.be/AO91eH0Gx0c	http://dx.doi.org/10.5258/SOTON/AI3SD0160	 Dr Tom Fleming *Arctoris*
	Machine Learning and AI for Drug Design	https://youtu.be/BP5j_h3CxW0	http://dx.doi.org/10.5258/SOTON/AI3SD0161	 Prof Ola Engkvist *AstraZeneca & Chalmers* University
	Accelerating design of organic materials with Machine Learning and AI	https://youtu.be/5SDEUFLYG-k	http://dx.doi.org/10.5258/SOTON/AI3SD0162	 Professor Olexandr Isayev – Carnegie Mellon University

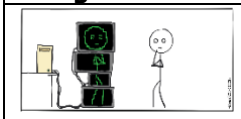
5. AI4SD Autumn Seminar V: Quantum Machine Learning

Image	Talk	Video Link	Link	Speaker
	Learning to Control Quantum Systems Robustly	https://youtu.be/8P-C5NUye_Q	http://dx.doi.org/10.5258/SOTON/AI3SD0163	 Dr Frank C Langbein *Cardiff University*
	The Variational Quantum Eigensolver – progress and near term applications for quantum chemistry	https://youtu.be/MfXqhQeSlN4	http://dx.doi.org/10.5258/SOTON/AI3SD0164	 Jules Tilly *Rahko & UCL*
	Quantum Machine Learning	https://youtu.be/AKsAYrl_E6I	http://dx.doi.org/10.5258/SOTON/AI3SD0165	 Prof Anatole von Lilenfeld *University of Vienna*

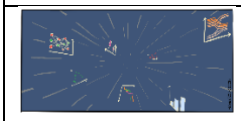
6. AI3SD Autumn Seminar VI: Medicinal Chemistry

Image	Talk	Video Link	Link	Speaker
	A vision of Medicinal Chemistry for the future	https://youtu.be/sJb7O5mUsXs	http://dx.doi.org/10.5258/SOTON/AI3SD0167	 Dr Lewis Vidler *UCB*
	What a Medicinal Chemist Needs to Know about Explainable Artificial Intelligence	https://youtu.be/1Ig5VIlrfe4	http://dx.doi.org/10.5258/SOTON/AI3SD0168	 Dr Alexander (Al) G. Dossetter *Medchemica Ltd*

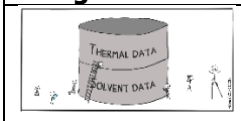
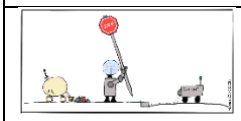
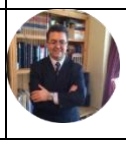
7. AI4SD Autumn Seminar VII: Digital Twins

Image	Talk	Video Link	Link	Speaker
	The Universal Digital Twin – accessing the world of Chemistry	https://youtu.be/4T3GN8WN8W8	http://dx.doi.org/10.5258/SOTON/AI3SD0169	 Prof Marcus Kraft *University of Cambridge*

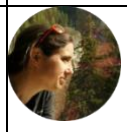
8. AI4SD Autumn Seminar VIII: Molecules, Graphs & Networks

Image	Talk	Video Link	Link	Speaker
	Chemical Space Exploration	https://youtu.be/J1ZXr3w7eps	http://dx.doi.org/10.5258/SOTON/AI3SD0170	 Prof Jan Jensen *University of Copenhagen*
	The hyperparameter optimisation of graph neural networks for molecular property prediction	https://youtu.be/qfkQ3-G2G6M	http://dx.doi.org/10.5258/SOTON/AI3SD0171	 James Yuan *Heriot Watt University*

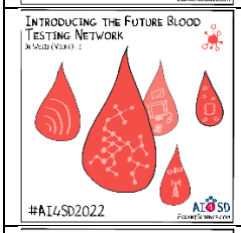
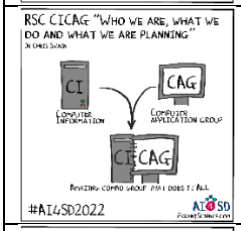
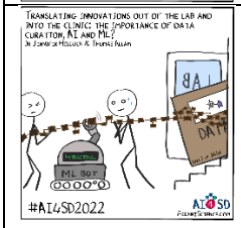
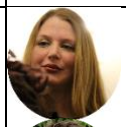
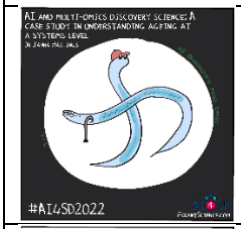
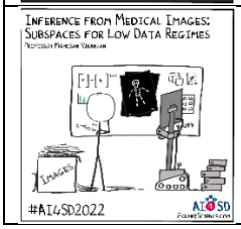
9. AI4SD Autumn Seminar VIII: Molecules, Graphs & Networks

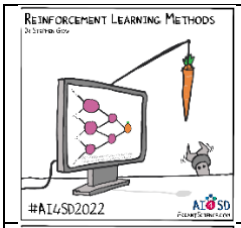
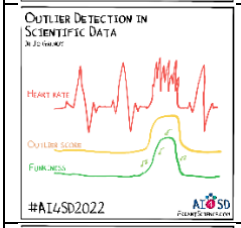
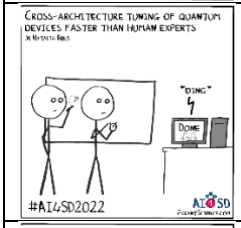
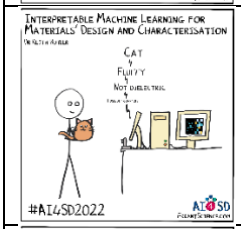
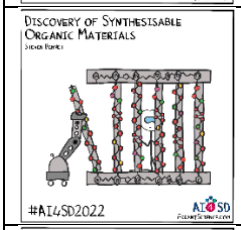
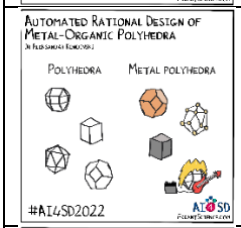
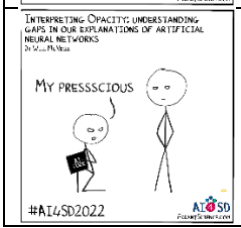
Image	Talk	Video Link	Link	Speaker
	Audacity of huge: Machine Learning for the discovery of transition metal catalysts and materials	https://youtu.be/QnIkM28h0iU	http://dx.doi.org/10.5258/SOTON/AI3SD0172	 Prof Heather Kulik *MIT*
	Artificial Intelligence for Safer Urban Spaces	https://youtu.be/rQRmEI44wCw	http://dx.doi.org/10.5258/SOTON/AI3SD0173	 Prof Zoheir Sabeur *University of Bournemouth*

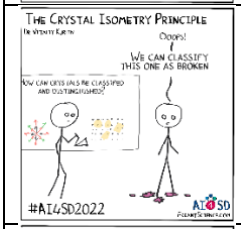
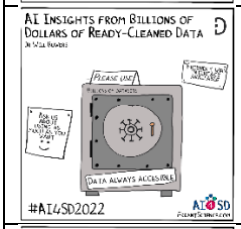
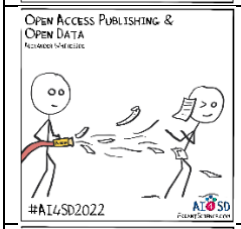
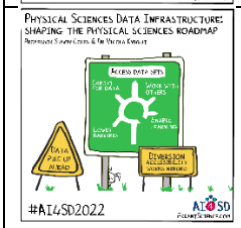
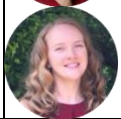
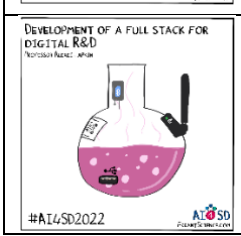
10. AI4SD Autumn Seminar VIII: Molecules, Graphs & Networks

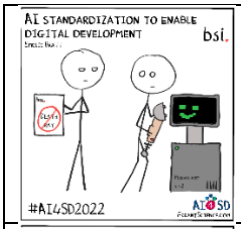
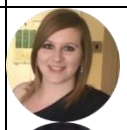
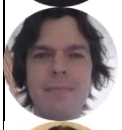
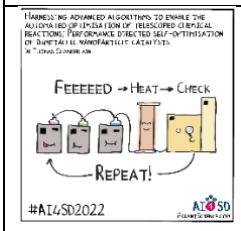
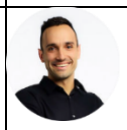
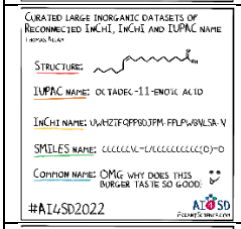
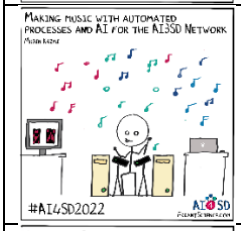
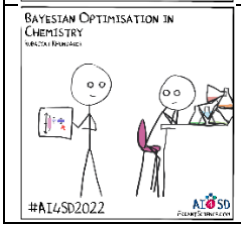
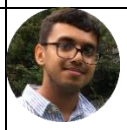
Image	Talk	Video Link	Link	Speaker
	Data Driven Molecular Design	https://youtu.be/l4s7Bnk0VdY	http://dx.doi.org/10.5258/SOTON/AI3SD0174	 Dr Barbara Zdrazil *EMBL-EBI & University of Vienna*
	Finding Small Molecules and their Metabolites in Big Data	https://youtu.be/-0HlT3qMMtQ	http://dx.doi.org/10.5258/SOTON/AI3SD0175	 Associate Prof Emma Schymanski *University of Luxembourg*

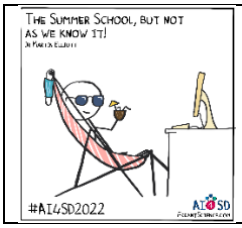
A.2.8. AI4SD Conference

Image	Talk	Video Link	DOI Link	Speaker
	Welcome & AI4SD Retrospective	https://youtu.be/VFk654w9Rgc	N/A	 Prof Jeremy Frey *University of Southampton*
	Introducing the Future Blood Testing Network	https://youtu.be/z5KYxBYshtU	http://dx.doi.org/10.5258/SOTON/AI3SD0185	 Dr Weizi (Vicky) Li *University of Reading*
	RSC CICAG "Who we are, what we do and what we are planning"	https://youtu.be/F4WBAq_2HIQ	http://dx.doi.org/10.5258/SOTON/AI3SD0186	 Dr Chris Swain *Cambridge MedChem Consulting*
	Equality, Diversity, Inclusion in Networks: Developing your inclusive approach	https://youtu.be/9_Zs890TvhM	http://dx.doi.org/10.5258/SOTON/AI3SD0187	 Debra Fearnshaw *University of Nottingham*
	Translating innovations out of the lab and into the clinic: the importance of data curation, AI and ML?	https://youtu.be/ProK7XWc6Qc	http://dx.doi.org/10.5258/SOTON/AI3SD0188	  Dr Jennifer Hiscock *University of Kent* Thomas Allam *University of Southampton*
	AI and multi-omics discovery science: A case study in understanding ageing at a systems level	https://youtu.be/HuunKNZdVPk	http://dx.doi.org/10.5258/SOTON/AI3SD0189	 Dr Janna Hastings *EFPL/UNIL & UCL*
	Inference from Medical Images: Subspaces for Low Regimes	https://youtu.be/uGLfHCZRe78	http://dx.doi.org/10.5258/SOTON/AI3SD0190	 Prof Mahesan Niranjan *University of Southampton*

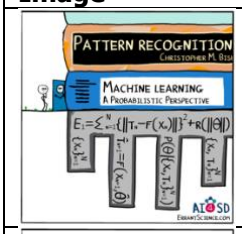
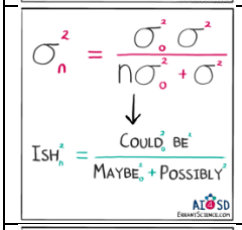
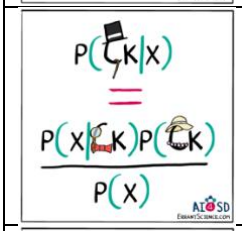
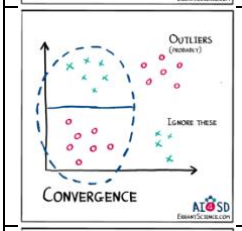
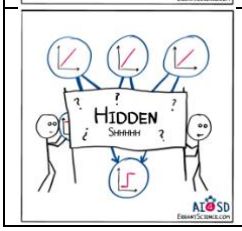
	Reinforcement Learning Methods	https://youtu.be/G0RSuABpIaA	http://dx.doi.org/10.5258/SOTON/AI3SD0191		Dr Stephen Gow *University of Southampton*
	Outlier Detection in Scientific Data	https://youtu.be/MhaJ2IZ2IBc	http://dx.doi.org/10.5258/SOTON/AI3SD0192		Dr Jo Grundy *University of Southampton*
	Cross-architecture tuning of quantum devices faster than human experts	https://youtu.be/yZwCpJTRuqA	http://dx.doi.org/10.5258/SOTON/AI3SD0193		Dr Natalia Ares University of Oxford
	Interpretable Machine Learning for Materials' Design and Characterisation	https://youtu.be/emx_82kTm-M	http://dx.doi.org/10.5258/SOTON/AI3SD0194		Dr Keith Butler *STFC*
	AI and optimisation in Computational Chemistry	https://youtu.be/enFSHTdc71k	http://dx.doi.org/10.5258/SOTON/AI3SD0195		Dr Grant Hill *University of Sheffield*
	Discovery of Synthesisable Organic Materials	https://youtu.be/3rjyMy4Ajfw	TBC		Steven Bennett *Imperial College London*
	Automated Rational Design of Metal-Organic Polyhedra	https://youtu.be/-nNTxYTFpKo	http://dx.doi.org/10.5258/SOTON/AI3SD0197		Dr Aleksandar Kondinski *University of Cambridge*
	Interpreting Opacity: understanding gaps in our explanations of artificial neural networks	https://youtu.be/IkuSWhQRWro	TBC		Dr Will McNeill *University of Southampton*

	Event detection in a single-molecule data how to find molecule data how to find molecular signatures without (too many) prior assumptions	https://youtu.be/J44UwGE6od4	http://dx.doi.org/10.5258/SOTON/AI3SD0199		Professor Tim Albrecht *University of Birmingham*
	Making sense of highly flexible molecular simulations: Where AI can help and where not	https://youtu.be/mJ652138x0k	http://dx.doi.org/10.5258/SOTON/AI3SD0200		Dr Christof Jager *University of Nottingham*
	The crystal Isometry Principle	https://youtu.be/20ywx3x8Zqc	http://dx.doi.org/10.5258/SOTON/AI3SD0203		Dr Vitaliy Kurlin *University of Liverpool*
	AI Insight from Billions of Dollars of Ready-Cleaned Data	https://youtu.be/Qhu27A1kuik	TBC		Dr Will Bowers *Dotmatics*
	Open Access Publishing & Open Data	https://youtu.be/oNFoSaPL1vo	http://dx.doi.org/10.5258/SOTON/AI3SD0204		Dr Alexander Whiteside *Digital Discovery RSC*
	Sharing Data Science Solutions Across Domain via Patterns	https://youtu.be/ByfJdCILx38	http://dx.doi.org/10.5258/SOTON/AI3SD0205		Dr Gary Gustafson *CAS*
	Physical Sciences Data Infrastructure: shaping the physical sciences roadmap	https://youtu.be/4Ukn7TawAhs	http://10.0.20.138/SOTON/AI3SD0208	 	Prof Simon Coles & Dr Nicola Knight *University of Southampton*
	Development of a full stack for digital R&D in chemistry and chemical process development	https://youtu.be/DXArgm5VtRo	https://youtu.be/DXArgm5VtRo		Professor Alexei Lapkin *University of Cambridge*

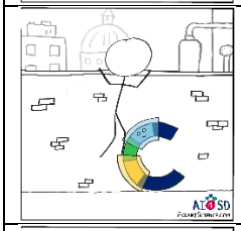
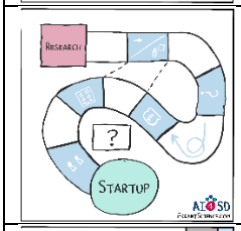
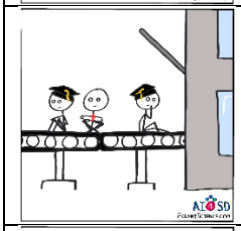
	AI standardization to enable digital development	https://youtu.be/lyJUMuKoZiw	http://10.0.20.138/SOTON/AI3SD0210	 Emelie Bratt *BSI*
	AI4SD & IoFT for Ethics Working Group Introducing the Working Group & Our Methodologies: Moral IT Cards & Design Fiction	https://youtu.be/5-aJe_feCTo	http://10.0.20.138/SOTON/AI3SD0211	 Dr Samantha Kanza *University of Southampton*  Dr Peter Craigon *University of Nottingham*  Dr Naomi Jacobs *Lancaster University*
	Harnessing advanced algorithms to enable the automated optimisation of telescoped chemical reactions; Performance directed self-optimisation of bimetallic nanoparticle catalysts	https://youtu.be/3pwBL_KKvIc	http://10.0.20.138/SOTON/AI3SD0212	 Dr Thomas Chamberlain *University of Leeds*
	High-throughput generation of chemical isomers for the development of molecular models of biocrude oils	https://youtu.be/SC-KsfdIOw8	http://10.0.20.138/SOTON/AI3SD0213	 Dr Francisco Martin-Martinez *Swansea University*
	Curated large inorganic datasets of Reconnected InChI, InChi and IUPAC name	https://youtu.be/WvBJJu5HK5c	http://10.0.20.138/SOTON/AI3SD0214	 Thomas Allam *University of Southampton*
	Making music with automated processes and AI for the AI3SD Network	https://youtu.be/hRKajxfoIRY	http://10.0.20.138/SOTON/AI3SD0215	 Mubin Kazmi *University of Southampton*
	Bayesian Optimisation in Chemistry	https://youtu.be/Wec-95iEDN4	http://10.0.20.138/SOTON/AI3SD0216	 Rubaiyat Khondaker *University of Cambridge*

	The Summer School, but not as we know it!	https://youtu.be/dB2pvluvuJU	http://10.0.20.138/SOTON/AI3SD0217	 Dr Martin Elliot *Kings College London*

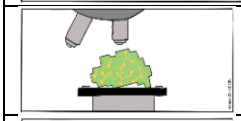
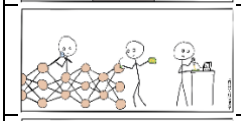
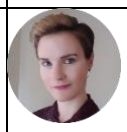
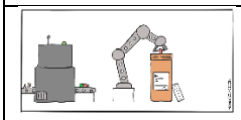
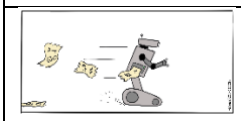
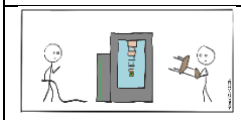
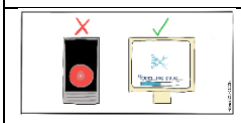
A.2.9. AI4SD Machine Learning Summer School

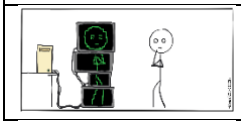
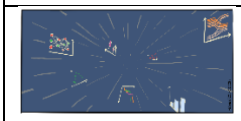
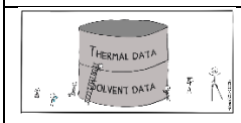
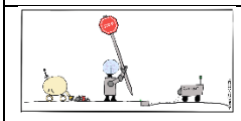
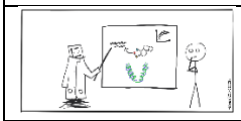
Image	Talk	Video Link	DOI Link	Speaker
	ML1: Mathematical Foundations for ML	https://youtu.be/1__M_wVeoZA	http://dx.doi.org/10.5258/SOTON/AI3SD0262	 Professor Mahesan Niranjan *University of Southampton*
	ML2: Estimation with Machine Learning	https://youtu.be/tlzvW8I0x-8	http://dx.doi.org/10.5258/SOTON/AI3SD0263	 Professor Mahesan Niranjan *University of Southampton*
	ML3: Classification and Clustering	https://youtu.be/6JgRHath6K4	http://dx.doi.org/10.5258/SOTON/AI3SD0264	 Professor Mahesan Niranjan *University of Southampton*
	ML4: Linear Regression to Perceptron Convergence	https://youtu.be/nTL2r1bo6Ew	http://dx.doi.org/10.5258/SOTON/AI3SD0265	 Professor Mahesan Niranjan *University of Southampton*
	ML5: Radial Basis Functions and Multi-Layer Perceptrons	https://youtu.be/wfDagIcCcAY	http://dx.doi.org/10.5258/SOTON/AI3SD0266	 Professor Mahesan Niranjan *University of Southampton*

A.2.10. AI4SD ECR Series 2022

Image	Talk	Video Link	DOI Link	Speaker
	Introduction to EPSRC and Funding Opportunities	https://youtu.be/FIyS9PqIPhU	https://doi.org/10.5258/SOTON/AI3SD0256	 Dr Liam Boyle *EPSRC*
	Opportunities for ECRs in the Royal Society of Chemistry	https://youtu.be/SKmGx4WbdJQ	https://doi.org/10.5258/SOTON/AI3SD0257	 Robert Bowles *RSC*
	Research to Startup	https://youtu.be/Vll6fudjlvk	https://doi.org/10.5258/SOTON/AI3SD0258	 Mr Samuel Munday *University of Southampton*
	Transitioning to Industry: A long, Short Road	https://youtu.be/2SnPGw2cLuM	https://doi.org/10.5258/SOTON/AI3SD0259	 Will Bowers *Dotmatics*
	Create a Killer CV	https://youtu.be/2MwBZj_XLfc	https://doi.org/10.5258/SOTON/AI3SD0260	 Robert Bowles *RSC*
	Introduction to equality, diversity	https://youtu.be/La_ZlVYT5qo	https://doi.org/10.5258/SOTON/AI3SD0261	 Debra Fearnshaw *University of Nottingham*

A.3. Q & A's

Image	Talk	Link	Speaker
	Automated Chemical Oncology Expansion	http://dx.doi.org/10.5258/SOTON/AI3SD0154	 Dr Janna Hastings Otto-von-Guericke *University & UCL*
	Towards Biological Plausibility Using Linked Open Data	http://dx.doi.org/10.5258/SOTON/AI3SD0155	 Dr Egon Willghagen *Masstricht University*
	How can Explainable AI help scientific exploration	http://dx.doi.org/10.5258/SOTON/AI3SD0156	 Prof Carlos Zednik Eindhoven *University of Technology*
	Explainable Machine Learning for Trustworth	http://dx.doi.org/10.5258/SOTON/AI3SD0157	 Dr Fosca Giannotti *University of Pisa*
	Statistics Are a Girl's Best friend: Expanding the mechanistic Study Toolbox with Data Science	http://dx.doi.org/10.5258/SOTON/AI3SD0158	 Dr Anat Milo Ben-*Gurion University of Negev*
	Data management: at the root of high-throughput experimentation	http://dx.doi.org/10.5258/SOTON/AI3SD0159	 Dr Nessa Carson *Syngenta*
	Machine Learning and AI for Drug Design	http://dx.doi.org/10.5258/SOTON/AI3SD0161	 Prof Ola Engkvist *AstraZeneca & Chalmers University*
	Accelerating design of organic materials with Machine Learning and AI	http://dx.doi.org/10.5258/SOTON/AI3SD0162	 Prof Olexandr Isayev *Carnegie Mellon University*
	Learning to Control Quantum Systems Robustly	http://dx.doi.org/10.5258/SOTON/AI3SD0163	 Dr Frank C Langbein *Cardiff University*
	The Variational Quantum Eigensolver progress and near term applications for quantum chemistry	http://dx.doi.org/10.5258/SOTON/AI3SD0164	 Jules Tilly *Rahko & UCL*
	Quantum Machine Learning	http://dx.doi.org/10.5258/SOTON/AI3SD0165	 Professor Anatole von Lilenfeld *University of Vienna*
	A vision of Medicinal Chemistry for the future	http://dx.doi.org/10.5258/SOTON/AI3SD0167	 Dr Lewis Vidler *UCB*
	What a Medicinal Chemist Needs to Know about	http://dx.doi.org/10.5258/SOTON/AI3SD0168	 Dr Alexander (Al) G. Dossetter *Medchemica Ltd*

	Explainable Artificial Intelligence		
	The Universal Digital Twin – accessing the world of Chemistry	http://dx.doi.org/10.5258/SOTON/AI3SD0169	 Prof Marcus Kraft *University of Cambridge*
	Chemical Space Exploration	http://dx.doi.org/10.5258/SOTON/AI3SD0170	 Prof Jan Jensen *University of* Copenhagen
	The hyperparameter optimisation of graph neural networks for molecular property prediction	http://dx.doi.org/10.5258/SOTON/AI3SD0171	 James Yuan *Heriot Watt University*
	Audacity of huge: Machine Learning for the discovery of transition metal catalysts and materials	http://dx.doi.org/10.5258/SOTON/AI3SD0172	 Prof Heather Kulik MIT
	Artificial Intelligence for Safer Urban Spaces	http://dx.doi.org/10.5258/SOTON/AI3SD0173	 Prof Zoheir Sabeur *University of Bournemouth*
	Data Driven Molecular Design	http://dx.doi.org/10.5258/SOTON/AI3SD0174	 Dr Barbara Zdrazil *EMBL-EBI & University of Vienna*
	Finding Small Molecules and their Metabolites in Big Data	http://dx.doi.org/10.5258/SOTON/AI3SD0175	 Associate Prof Emma Schymanski *University of Luxembourg*

A.4. Humans of AI4SD Interview Series

Title	Interviewer
Humans-of-AI4SD-Interview-1: Professor Andy Stanford-Clark	Michelle Pauli
Humans-of-AI4SD-Interview-2: Professor John Overington	Dr Wendy Warr
Humans-of-AI4SD-Interview-3: Professor Jonathan Goodman	Prof Jeremy Frey
Humans-of-AI4SD-Interview-4: Dr Naomi Jacobs	Dr Samantha Kanza
Humans-of-AI4SD-Interview-5: Dr Reinhard Maurer	Michelle Pauli
Humans-of-AI4SD-Interview-6: Professor Matthew Todd	Michelle Pauli
Humans-of-AI4SD-Interview-7: Professor Tim Albrecht	Michelle Pauli
Humans-of-AI4SD-Interview-8: Dr Jennifer Hiscock	Michelle Pauli
Humans-of-AI4SD-Interview-9: Dr Nicholas Watson	Michelle Pauli
Humans-of-AI4SD-Interview-10: Dr Martin Immanuel-Bittner	Michelle Pauli
Humans-of-AI4SD-Interview-11: Dr Simone Vannuccini	Michelle Pauli
Humans-of-AI4SD-Interview-12: Ms Ekaterina Prytkova	Michelle Pauli
Humans-of-AI4SD-Interview-13: Dr Louise Dennis	Michelle Pauli
Humans-of-AI4SD-Interview-14: Dr Zosia Beckles	Michelle Pauli
Humans-of-AI4SD-Interview-15: Dr Keith Butler	Michelle Pauli
Humans-of-AI4SD-Interview-16: Dr James Cumby	Michelle Pauli
Humans-of-AI4SD-Interview-17: Dr Tehri Nurmikko-Fuller	Michelle Pauli
Humans-of-AI4SD-Interview-18: Dr Mark Warne	Michelle Pauli
Humans-of-AI4SD-Interview-19: Dr Paul Dingwall	Michelle Pauli
Humans-of-AI4SD-Interview-20: Dr Grant Hill	Michelle Pauli
Humans-of-AI4SD-Interview-21: Dr Al Dossetter	Michelle Pauli
Humans-of-AI4SD-Interview-22: Dr Aurora Clark	Michelle Pauli
Humans-of-AI4SD-Interview-23: Dr Barbara Zdrazil	Michelle Pauli
Humans-of-AI4SD-Interview-24: Professor Carlos Zednik	Michelle Pauli
Humans-of-AI4SD-Interview-25: Egon Willighagen	Michelle Pauli
Humans-of-AI4SD-Interview-26: Professor Charlotte Deane	Michelle Pauli
Humans-of-AI4SD-Interview-27: Christopher Gutteridge	Michelle Pauli
Humans-of-AI4SD-Interview-28: Dr Will McNeill	Michelle Pauli
Humans-of-AI4SD-Interview-29: Professor Tony Hey	Michelle Pauli
Humans-of-AI4SD-Interview-30: Professor Henry Rzepa	Michelle Pauli
Humans-of-AI4SD-Interview-31: Dr Frank Langbein	Michelle Pauli
Humans-of-AI4SD-Interview-32: Dr Heather Kulik	Michelle Pauli
Humans-of-AI4SD-Interview-33: Dr Jan Jensen	Michelle Pauli
Humans-of-AI4SD-Interview-34: Jules Tilly	Michelle Pauli
Humans-of-AI4SD-Interview-35: Professor Markus Kraft	Michelle Pauli
Humans-of-AI4SD-Interview-36: Dr Nessa Carson	Michelle Pauli
Humans-of-AI4SD-Interview-37: Yingfang Yuan	Michelle Pauli
Humans-of-AI4SD-Interview-38: Professor Zoheir Sabeur	Michelle Pauli

A.5. Posters

A.5.1. AI4SD 1st Conference 2019

Poster Title	Name
Ontologies for Chemistry	Dr Colin Batchelor – Royal Society of Chemistry
The Physical Sciences Data-Science Service	Dr Nicola Knight – University of Southampton
Translation level regulation of cellular protein concentrations	Mrs Pratheeba Jeyananthan – University of Jaffna
Machine Learning with Coarse-Grained Molecules to Determine Thermodynamic Properties	Mr Kezheng Zhu – Imperial College London
Saliency Map on Cnns for Protein Secondary Structure Prediction	Mr Guillermo Romero Moreno – University of Southampton
Transfer Learning Across Species on Single Cell Datasets Using a Neural Network	Miss Xin Du
Predictive Modelling of Post-Translational Regulation During Human Cell Cycle Progression	Mr Gregory Parkes – University of Southampton
Robust Subspace Methods for Anomaly Detection in High Dimensional Datasets	Mr Omar Shetta – University of Southampton
Machine–Learning-Based Density Functional Tight Binding Parametrisation for Hybrid Organic-Metallic Systems	Dr Adam McSloy – University of Bremen

A.5.2. AIReact 2020

Poster Title	Name
Industrialising X-Ray Fragment Hit Progression	Anthony Aimon – Diamond Light Source Ltd
Reaction InChI (RInChI): Present and Future	Gerd Blanke – StructurePendium Technologies GmbH
Development of an automated gas phase catalytic microreactor platform for kinetic studies	Solomon Gajere Bawa UCL
Active Learning for Cost-Efficient Reaction Prediction using Kinetic Data	Paul Dingwall – Queens University Belfast
Catalyst Seeking Substrate: Computational Prediction in Homogeneous Organometallic Catalysis	Derek James Durand – University of Bristol
RetroBiocat: a tool for computer aided synthesis planning of biocatalytic cascades	William Finnigan – University of Manchester
Predicting Cytochrome P450 Sites of Metabolism	Elena Gelžinyté – University of Cambridge
What data is really needed for the synthesis routes' prediction and why data preparation is still a bottleneck?	Elena Herzog – Elsevier
A Platform for Automating Catalytic Chemical Synthesis to Understand a Complex Pd-Catalysed Reaction System Using Data Analysis, Mechanistic Studies and Reaction Optimisation	Christopher Horbaczewskyj – University of York
Atom-To-Atom Mapping: A Benchmarking Study	Arkadii Lin – University of Strasbourg
Formation of artificial cells with distributed cores as multi-functional microreactors using 3D-printed microfluidics	Jin Li and David Barrow – Cardiff University

Reaxys Predictive Retrosynthesis (PAI): rewiring chemistry and redesigning synthetic routes	Elliott Parris – Elservier
Computational Methods to Identify Novel Medicinal Chemistry Relevant Heterocycles	Fergus Preston – Drug Discovery Unit, University of Dundee
A comprehensive modeling methodology for the development of QSPR models for kinetic characteristics of chemical reactions	Assima Rakhimbekova – Kazan Federal University
Catalyst Design via Machine Learning	Stamatia Zavitsanou – Oxford University
Artificial Labels for Multi-label Training of Neural Networks Policies for Retro-Synthetic Template Selection and Route Finding	Esben Jannik Bjerrum – AstraZeneca
AI/Machine Learning for Chemical Development	David Buttar – AstraZeneca

A.5.3. Skills4Scientists July 2021

Poster Title	**Name**
Nearer the nearsightedness principle: Large-scale quantum chemical calculations	András Vékássy – University of Southampton
Generation of isomers for fast development of molecular datasets	Anna Catton – Swansea University
Combining Ultrasonic Methods and Machine Learning Techniques to Assess Baked Products Quality	E. Gulset; D.E. Morrie; S Grebby; A. Ibrahim; N.J.Watson – University of Nottingham
Interactive Knowledge-Based Solvent Selection Tool	Hewan Zewdu – University of Nottingham
CV in High Throughput Chemistry	Jamie Longio & Reid Research Group – University of Strathclyde
A deep convolutional neural network for real-time full profile analysis of big powder diffraction data	H. Dong – UCL; K. Butler – Rutherford Laboratory; R. Khatry – National Physical Laboratory; S.D.M Jacques –Finden Limited; A.M.Beales – UCL & Finden Limited; A. Vamvakeros – UCL & Finden Limited
Relative Structural Analysis on Molecular Perovskite	Kevin Daniel Calvache Ramos – Queen Mary University London
Structure-activity relationship analysis of supramolecular antimicrobials	Kaylee Patel – The University of Manchester; Dr. Cally Haynes – UCL; Dr Jennifer Hiscock – University of Kent; Samuel Munday – University of Southampton
Dewetting in Thin Liquid Films: Using Sparse Optimization to Learn Evolution Equations	Aspen Fenzel – University of Sheffield; Professor Nigel Clarke – University of Sheffield
Latent Space encoding of Molecular Crystal Structure	Wong King Ming Alex – University of Southampton
Continuous Flow Chemical Process Self-Optimisation by Machine Learning	Louis Greenhalgh & Chamberlain Group – University of Leeds
Creating a merged dataset and its exploration with different Machine Learning algorithms	Maximilian Hoffmann – Freie Universität Berlin
Machine learning of quantum mechanical lattice energies for molecular crystal structure prediction	Rebecca J Clements – University of Southampton
Bayesian optimisation in Chemistry	Rubaiyat Khondaker – University of Cambridge; Stephen Gow – University of Southampton; Mahesan Niranjan – University of Southampton; Jeremy Frey – University of Southampton

A deep neural network for generation of functional organic materials	Rhyan Barrett – University of Warwick; Julia Westermayr – University of Leipzip; Reinhard Maurer – University of Warwick
Curating inorganic chemical datasets to train RNN and transformer ML models to predict IUPAC names from InChI	Thomas Allam – University of Southampton
Learning the crystallographic phase problem	Sarah Scripps – University of Edinburgh; Dr James Cumby – University of Edinburgh; Dr Sohan Seth – University of Edinburgh
Exploring coherent diffractive imaging using AI	Gavin Man – University of Oxford

Appendix B. Funded Project Reports

This section will detail the reports from funded projects: Pilot Projects, Intern Projects and Summer School Projects.

B.1. Pilot Project Series Reports

Project	Link	Principal Investigator & Project Partners
Predicting the Activity of Drug Candidates where this is No Target.	http://dx.doi.org/10.5258/SOTON/P0085	Professor Matthew Todd – University College London; Auromind; ExScientia; Intellegens
'Next-next' Generation Quantum DNA Sequencing with Chemical Surface Design and Capsule Nets	http://dx.doi.org/10.5258/SOTON/P0036	Professor Tim Albrecht, University of Birmingham; City, University of London
Deep Learning enhanced quantum chemistry: Pushing the limits of Materials Discovery	http://dx.doi.org/10.5258/SOTON/P0041	Dr Reinhard J. Maurer – University of Warwick; University of Strathclyde; Carnegie Mellon University
Optimising Flatland: Inverse design of desalination membranes	http://dx.doi.org/10.5258/SOTON/P0040	Dr J. Grant Hill – University of Sheffield; Imperial College London
Interpretable crystal descriptions across length scales for materials discovery	http://dx.doi.org/10.5258/SOTON/P0038	Dr Paul Dingwall – Queens University Belfast
Artificial Intelligence for reconstruction and super-resolution of chemical tomography	http://dx.doi.org/10.5258/SOTON/P0037	Dr Keith Butler – STFC; Finden Ltd

B.2. Intern Series Reports

Title	Link	Intern Student
A deep neural network for generation of functional organic molecules	http://dx.doi.org/10.5258/SOTON/AI3SD0145	Rhyan Barrett – University of Warwick
Optimising Ag/Au Alloyed Nanoparticle Catalysts in Continuous Flow; Discrete vs. Continuous Variable Optimisation	http://dx.doi.org/10.5258/SOTON/AI3SD0146	Louis Greenhalgh – University of Leeds
Machine Learning Physics Models for Materials Self-Assembly	http://dx.doi.org/10.5258/SOTON/AI3SD0139	Aspen Fenzl – University of Sheffield
Relative Structural Analysis on Molecular Pervoskite	http://dx.doi.org/10.5258/SOTON/AI3SD0147	Kevin Calvache – Queen Mary University London
Curating a chemical dataset to train recurrent neural network models to predict IUPAC name from InChI's	http://dx.doi.org/10.5258/SOTON/AI3SD0148	Thomas Allam – University of Southampton
Learning the Crystallographic Phase Problem	http://dx.doi.org/10.5258/SOTON/AI3SD0142	Sarah Jane Scripps – University of Edinburgh
Latent Space Encoding of Molecular Crystal Structure	http://dx.doi.org/10.5258/SOTON/AI3SD0150	Wong King Ming Alex – University of Southampton
High-throughput generation of structural isomers for fast development of molecular datasets to train machine learning algorithms	http://dx.doi.org/10.5258/SOTON/AI3SD0141	Anna Catton – University of Swansea
Nearer the nearsightedness principle: Large-scale quantum chemical calculations	http://dx.doi.org/10.5258/SOTON/AI3SD0140	András Vékássy – University of Southampton

B.3. Summer School Reports

Title	Link	Students
Group 1: Challenge: Task 1 – Predict Solubility Given a Large Set of Calculated Features	http://dx.doi.org/10.5258/SOTON/AI3SD0244	Jonathan Swan – University of Cambridge; Bradley Patrick – Nottingham Trent University; Andrew Frisco – UCL; Dan Criveanu – University of Nottingham
Group 2: Challenge: Task 3 – Detect Defects in Electron Microscopy Images	https://doi.org/10.5258/SOTON/AI3SD0245	Ross J. Urquhard – University of Strathclyde; Chris Woodley – University of Liverpool; Katerina Karoni – University of Edinburgh; Jan Elsner – UCL; Daniel York – Swansea University
Group 5: Challenge: Nanopore "Defect Detection in Graphene Sheets"	http://dx.doi.org/10.5258/SOTON/AI3SD0246	Anna Bachs Herrera – Swansea University; Abdoulatif Cisse – University of Liverpool; Emilio Alexis de la Cruz Nunez Andrade – Swansea University; Philipp Deussen – UCL; Ivan Yankov – University of Strathclyde
Group 6: Challenge: Task 3 – Detect Defects in Electron Microscopy Images	http://dx.doi.org/10.5258/SOTON/AI3SD0247	Robert Dickson; Ben Honore; Hai Lin; Rachael Pirie
Group 7: Challenge 3 – Defect Detection in Graphene Sheets	http://dx.doi.org/10.5258/SOTON/AI3SD0248	James Osborne – University of Liverpool; Ellie Nelson – University of York; Edvin Mamo – University College Dublin; Shaoqi Zhan – University of Oxford; Steven Tendyra – University of Manchester
Group 8: Challenge: Event Detection in Nanopore Data	http://dx.doi.org/10.5258/SOTON/AI3SD0249	Wole Ademola Adewole – University of Southampton; Halil Ibrahim Aysel – University of Southampton; Stephen Gow – University of Southampton; Zheng Jiang – University of Southampton; Dimitrios Stamatis – University of Southampton
Group 14: Challenge: Defect Detection in Graphene Sheets	http://dx.doi.org/10.5258/SOTON/AI3SD0250	Peng Bao – University of Liverpool; Jack Macklin – University of Bath; Masood Gheasi – University of Southampton
Group 16: Challenge: Task 3 – Detect Defects in Electron Microscopy Images	http://dx.doi.org/10.5258/SOTON/AI3SD0251	Xuerui Guo – University of Southampton; Zien Ma – Cardiff University; Jayanta Kumar Pal – University of Liverpool

Appendix C. Journal and Conference Papers

The following journal and conference papers have been published as a result of AI4SD support:

1. Kanza, S. and Frey, J.G., 2019. A new wave of innovation in Semantic web tools for drug discovery. *Expert Opinion on Drug Discovery*, *14*(5), pp.433-444.
2. Kanza, S. and Frey, J.G., 2020. Semantic technologies in drug discovery—potential, practical, possibilities.
3. Kanza, S., Bird, C.L., Niranjan, M., McNeill, W. and Frey, J.G., 2021. The AI for Scientific Discovery Network+. *Patterns*, *2*(1), p.100162.
4. Tse, E.G., Aithani, L., Anderson, M., Cardoso-Silva, J., Cincilla, G., Conduit, G.J., Galushka, M., Guan, D., Hallyburton, I., Irwin, B.W. and Kirk, K., 2021. An Open Drug Discovery Competition: Experimental Validation of Predictive Models in a Series of Novel Antimalarials. *Journal of Medicinal Chemistry*, *64*(22), pp.16450-16463.
5. Dong, H., Butler, K.T., Matras, D., Price, S.W., Odarchenko, Y., Khatry, R., Thompson, A., Middelkoop, V., Jacques, S.D., Beale, A.M. and Vamvakeros, A., 2021. A deep convolutional neural network for real-time full profile analysis of big powder diffraction data. *npj Computational Materials*, *7*(1), pp.1-9.
6. Jacobs, N., Brewer, S., Craigon, P.J., Frey, J., Gutierrez, A., Kanza, S., Manning, L., Munday, S., Pearson, S. and Sacks, J., 2021. Considering the ethical implications of digital collaboration in the Food Sector. *Patterns*, *2*(11), p.100335.
7. Gutteridge, C., 2021. Data hygiene factors. *Patterns*, *2*(2), p.100207.
8. Kanza, S. and Knight, N.J., 2022. Behind every great research project is great data management. *BMC Research Notes*, *15*(1), pp.1-5.
9. Johnson, R., 2021. Artificial, augmented and automated chemistry. *Nature Chemistry*, *13*(9), pp.811-813.
10. Kanza, S., Willoughby, C., Bird, C.L. and Frey, J.G., 2022. eScience Infrastructures in Physical Chemistry. *Annual Review of Physical Chemistry*, *73*, pp.97-116.
11. Manning, L., Brewer, S., Craigon, P.J., Frey, J., Gutierrez, A., Jacobs, N., Kanza, S., Munday, S., Sacks, J. and Pearson, S., 2022. Artificial intelligence and ethics within the food sector: Developing a common language for technology adoption across the supply chain. *Trends in Food Science & Technology*.
12. Chandler-Wilde, S., Kanza, S., Fisher, O., Fearnshaw, D. and Jones, E., 2022. Reflections on an EDI Survey of UK-Government-Funded Research Networks in the UK.
13. Willoughby, C. and Frey, J.G., 2022. Data management matters. *Digital Discovery*.
14. Khondaker, R.M., Gow, S., Kanza, S., Frey, J.G. and Niranjan, M., 2022. Robustness under parameter and problem domain alterations of Bayesian optimization methods for chemical reactions. *Journal of Cheminformatics*, *14*(1), pp.1-10.
15. Gow, S., Niranjan, M., Kanza, S. and Frey, J.G., 2022. A review of reinforcement learning in chemistry. *Digital Discovery*.
16. Craigon, P.J., Sacks, J., Brewer, S., Frey, J., Mendoza, A.G., Jacobs, N., Kanza, S., Manning, L., Munday, S., Wintour, A. and Pearson, S., 2022. Ethics by Design: Responsible Research & Innovation for AI in the Food Sector. *Journal of Responsible Technology*, p.100051.
17. Jacobs, N., Brewer, S., Craigon, P.J., Frey, J., Gutierrez, A., Kanza, S., Manning, L., Munday, S., Pearson, S. and Sacks, J., 2021. Considering the ethical implications of digital collaboration in the Food Sector. *Patterns*, *2*(11), p.100335.
18. Manning, L., Brewer, S., Craigon, P.J., Frey, J., Gutierrez, A., Jacobs, N., Kanza, S., Munday, S., Sacks, J. and Pearson, S., 2022. Artificial intelligence and ethics within the food sector: Developing a common language for technology adoption across the supply chain. *Trends in Food Science & Technology*.
19. Craigon, P.J., Sacks, J., Brewer, S., Frey, J., Mendoza, A.G., Jacobs, N., Kanza, S., Manning, L., Munday, S., Wintour, A. and Pearson, S., 2022. Ethics by Design: Responsible Research & Innovation for AI in the Food Sector. *Journal of Responsible Technology*, p.100051.

Appendix D. Presentations & Posters about AI4SD

The following presentations were given about AI4SD at external events:

1. Dial-a-Molecule Annual Meeting – July 2019
2. IoFT Network+ Conference – September 2019
3. Future Labs Live – June 2022
4. The AI4SD Poster has also been presented at the following events:
    a. RSC Ultra Large Chemical Libraries Meeting – August 2022
    b. ELRIG Drug Discovery World 2022

Appendix E. Event Attendance

The table below shows the event attendance figures for our events and event series.

Date	Event	Registered	Attended	Attendance	No. Speakers
05/12/2018	AI3SD Network+ Launch	147	104	71%	6
22/01/2019	Network Town Meeting for Funding	28	17	61%	2
06/02/2019	Molecules Graphs & AI Workshop	30	22	73%	3
06/03/2019	AI in Drug Discovery & Drug Safety Workshop	44	32	76%	4
19/03/2019	AI for Materials Discovery Workshop	83	65	78%	5
01/05/2019	Semantics & Knowledge Learning for Chemical Design Workshop	23	17	74%	5
17/08/2019	AI & ML in Chemical Discovery & Development	30	27	90%	4
11/09/2019	AI3SD Network+ Town meeting & Funding Workshop	22	11	50%	4
12/09/2019	Machine Learning for Chemistry Training Workshop & Hackathon	27	23	85%	6
17/10/2019	AI Technologies for Allergen Detection & Smart Cleaning within Food Production	50	26	52%	3
06/11/2019	Quantum Computers: A Guide for the Perplexed	46	50	108%	1
18-19/11/2019	AI3SD Network+ Conference	102	80	78%	23
9-11/03/2020	AIReact2020	135	99	73%	29
Summer 2020	Summer Seminar Series	1231	735	60%	14
2020-2022	Data Seminar Series	358	184	51%	20
2021-2022	Winter Seminar Series	958	714	75%	18
Spring 2021	AI4Proteins	467	296	63%	14
Summer 2021	Skills4Scientists	740	558	75%	20
Summer 2021	ML4MC Summer School	34	33	97%	14
Winter 2021	Autumn Seminar Series	1103	669	61%	22
01-03/03/2022	AI4SD Conference 2022	116	99	85%	37
20-24/06/2022	ML Summer School	87	80	92%	5
25-26/07/2022	ECR Event	33	28	85%	6