

Conference Report

SCS Spring School on Digital Chemistry 2023

Part A: Getting Trained on Digital Chemistry in an Alpine Environment

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Spring School Goals and Mission

In recent years, we have seen an active shift towards data-driven decision-making in chemistry with the goal of accelerating drug-, crop protection-, and materials discovery. The rapid progress in this area of research is being driven by a growing open-source community as well as transdisciplinary collaboration in the fields of cheminformatics, machine learning, and molecular modeling.

Focus on Learning by Doing

With this Spring School, we wanted to provide the participants an opportunity to learn how to use this new technology for their own research. In addition to reviewing the fundamental concepts of machine learning, cheminformatics, and molecular modeling (Fig. 1), we introduced, in extensive hands-on sessions, the essential ingredients for a quicker adoption of data-driven solutions and more effective collaboration. The hands-on sessions focused both on the application of existing open-source toolkits and the acquisition of skills for the development of new technologies. The emphasis was on applications for drug and crop protection discovery.

Nearly half of the four-day seminar was dedicated to hands-on sessions (Fig. 2). With a team of 13 lecturers and coaches, we had an excellent staff-to-student ratio resulting in a very steep learning curve. With three exceptions, all instructors and coaches were from industry, *i.e.* from Idorsia, Syngenta, BASF, and IBM Research. See website for detailed information about the lecturers and coaches <https://aisem23.scg.ch>.

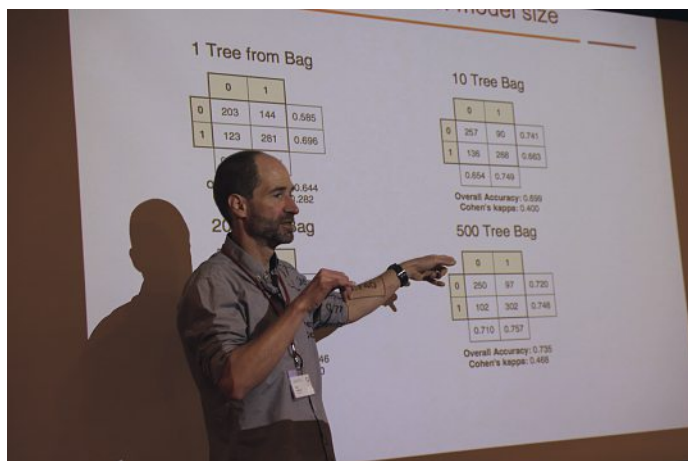


Fig. 1. Dr. Greg Landrum (ETH Zürich) in his lecture on Machine Learning Basics.



Fig. 2. Hands-on session: coaches and students.

Outlook

Thanks to the strong involvement from the supporting companies, and the financial support from Syngenta, Idorsia, the SCNAT and a few other sponsors, this event became possible and affordable for the student participants.

The body of students, 35 in total, was international (Switzerland, Germany, France, England and even California) and of diverse background (university students, but also two professors and several participants from industry). Sixteen posters were presented, followed by extensive scientific discussions, also outside the lecture hall.

This was the first SCS Seminar on this topic. Given its success and the very positive student feedback, the organizers are considering offering another edition of the Digital Chemistry Spring School. The wonderful Alpine scenery surrounding Les Diablerets and the fantastic venue, the Eurotel Victoria, with its nice staff, greatly contributed to a memorable experience.

Part B: The Students' Experience

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Introduction

The SCS Spring School on Digital Chemistry was an excellent opportunity for students and professionals to gather and learn about the latest trends and advancements in the field of digital chemistry (Fig. 3). The participants were able to see the state-of-the-art tools and developments in the field while networking with other students, post-docs, professors, and industry professionals.

Focus on Student Involvement

The students presented 16 posters over the span of two evenings. The available time provided all participants with the opportunity to engage in fruitful discussions about their research (Fig. 4). There were two juries to select the best presentations, a senior one consisting of lecturers and coaches, and a junior one consisting of participants.

But most of all, the students were actively involved in every lecture during the Spring School: All of them were followed by

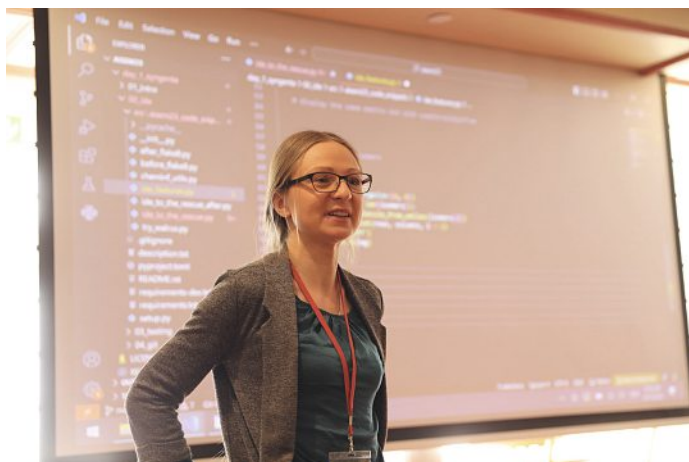


Fig. 3. Dr. Marzena Lehmann of Syngenta in her lecture on Technology Basics and Python Best Practice.



Fig. 4. Members of the two juries, Dr. Miriam Mathea (BASF; keynote lecturer), Rabia Ayub (University of York), and Dr. Greg Landrum (ETH Zürich) handing out the «special contributors' recognition» to Paula Linh Kramer of Saarland University.

a 2.5 hours long hands-on session where we had the opportunity to immediately put the acquired theoretical knowledge into practice. In the framework of these sessions, we could further our cheminformatics, computational and machine learning skills through a variety of exercises ranging from chemical data analytical coding tasks to fragment-based drug design to improve binding efficiency of ligands on protein targets. We also had a session where we developed a code in groups of eight to practice collaborating in teams. During these lectures we could acquire skills from experts that we can immediately transfer into our daily research.

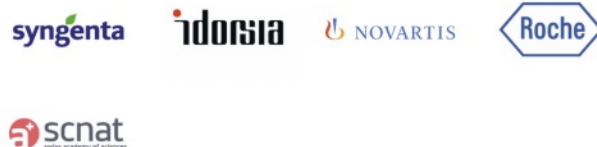
Conclusions

Looking back on this year's SCS Spring School on Digital Chemistry, participation has not only improved the technical skills of us students, but also provided an excellent opportunity to meet likeminded peers. The training in digital chemistry, with great introductory lectures, live hands-on exercises, and poster sessions was perfectly complemented by the social aspect of this event. This relaxed atmosphere encouraged participants to ask their questions, express constructive criticism, and to discuss with each other. This paved the way for the formation of networks which were further strengthened by the leisure activities provided. As a result, they came across new research topics, application areas for digital chemistry, while experiencing the

mesmerizing landscape of Switzerland. In conclusion, this event serves as a noteworthy example of how the natural sciences can extend beyond research and create opportunities for networking and personal growth.

Acknowledgements

We thank all our sponsors for their support as well as for their active involvement in this wonderful event.



Received: September 29, 2023