Programming for research - Ondřej Vávra and Jan Šťourač

The prize of the Dean of the Faculty of Science of Masaryk University was awarded to two researchers from the Protein Engineering team of the International Clinical Research Center of St. Anne's University Hospital Brno. In the category of the Best Student of the Doctoral Study Program, Ondřej Vávra and Jan Šťourač received it, as an evaluation and thanks for their work so far in the Loschmidt Laboratories of the Faculty of Science, Masaryk University and FNUSA-ICRC. On this occasion, we asked both colleagues who specializes in bioinformatics for a short interview.

I imagine bioinformatics as such IT guys in the laboratory. Is it true? And what have you already programmed in?

Ondřej: I probably wouldn't describe it that way, it's about a combination of IT and biology, but we are not programmers in laboratories například For example, I consider myself a self taught IT guy. I started at the high school, with Pascal. Then I worked in Bash, but in Loschmidt's labs I needed more complex scripts to process the data, so now I'm working in Python, where I'm still a slightly advanced user and I'm happy to be sitting in the office with Jan, who can help me.

Jan: In my case, it's more IT than biology or work in laboratories… I started programming in elementary school, my first programming "language" was Baltík and his simple programming of the wizard by graphical chaining of actions. At the gym I was a classic webmaker, so HTML, cascading styles, JavaScript, then PHP, SQL and in high school in the Pascal seminar. Currently, it's mainly Java for more complex applications and Python as a fast prototyping language.

So how did you get into Loschmidt's labs?

Ondřej: My journey was quite steep, I come from Hradec Králové and I had no idea about any Loschmidt laboratories. I chose to study at university mainly because of biology, which always attracted me the most. I got to Masaryk University, majoring in molecular biology. In the first semester, we had a seminar with the heads of all laboratories, where they presented their research activities. There I learned about Loschmidt's labs for the first time and I was very interested in the combination of IT and biology. And when I met structural biology in my sophomore year, it was decided. I have already done my bachelor's thesis here and I am satisfied here.

Jan: It was easier for me and a little earlier. Im from Brno and we had to take part in Secondary School professional activities at our gym. And in the search for a suitable topic, I was fascinated by bioinformatics as a fascinating connection between computer science and biology, and that was only a step to Masaryk University and Loschmidt's laboratories. I then continued working on the projects even after the completion of it and I have already stayed here.

What are your results during your time here and what are your next goals?

Ondřej: My probably biggest result is that I participated in the development of a method for rapid analysis of the passage of molecules through protein tunnels. We successfully performed several other analyzes with this method, thanks to an internship abroad, we established further cooperation, so we managed to evaluate it well. Three years ago, I also received the Brno Ph.D. The talent of the South Moravian Center for International Mobility (JCMM), however, I am now in the fourth year of doctoral studies, so it is most important for me to combine work here with writing a doctoral thesis. So the closest goal is to complete my project and finish it successfully.

Jan: I primarily deal with the design and development of bioinformatics tools and databases. And it can be said that in some way I have been involved in almost everyone who has come out of our lab in the last ten years, which is twelve or thirteen programs. What makes me most happy is that they are popular in the scientific community and are really used by thousands of scientists around the world. As for studying, I'm in my second year, so in a while I will have a state exam and then I'll see. And if the pandemic situation allows, I would like to go on an internship at the European Bioinformatics Institute in Great Britain this year. But now it's hard to plan anything, so it's hard to say how it will all turn out in the end.

The most difficult you have encountered in your work so far, and what obstacle do you face now?

Ondřej: It was a purely professional problem, within the project in foreign cooperation I needed to integrate a special kind of simulations, which we have not done here yet. Long story short - it took about a year before I managed to find and put into operation a usable method and everything finally worked out. Now I face another obstacle. So far, there is no reliable automated method that can decide whether a protein has a ligand binding site on the surface or inside. If this problem could be solved and we could use software tools to determine the nature of these places, it would be a huge step forward. Using machine learning, we could apply this knowledge to the entire protein database and then better design changes to proteins or ligands, which would have an impact not only on applications in medicine, but also in industry.

Jan: I deal with one very difficult matter somehow continuously. It is about the robustness of our programs. Our calculations are quite demanding and run simultaneously on many computers. And as we all know, from time to time one stops randomly working or responding, and this then leads to a false calculation failure, which is a problem. So we're working to keep the running task running as well as possible, and for example to restart automatically, without the user noticing anything and we have to apologize for the technical inconvenience. But this is more of a technical matter, from a scientific point of view, the biggest challenge for me at

the moment is the development of the PredicSNP Onco tool. It is a software aimed at the personalized treatment of children's cancer, which aims to analyze the effect of mutations found in the cancer tissue of a particular patient on the functioning of key proteins and their interaction with known drugs. The results obtained by us will then be used by physicians in deciding and preparing a suitable therapeutic plan.

What do bioinformatics say about the threats posed to us by filmmakers like Matrix or Terminator?

Ondřej: Probably nothing, we have fun like other viewers ⍰ I have no specific fear of any IT thing. I don't have an Internet of Things facility at home, but it's more of a question that I don't care so much. And if I want to adjust the household to some automatic mode, then in the first place I will deal with security, which is something that a lot of people forget. As far as machine learning is concerned, it's more of a question for Elon Musk or Bill Gates, where they are going to go, I've never thought about it. It will definitely affect our lives, for example, let's take semi-autonomous cars, so we will see what it will look like in ten years.

Jan: Rather than the plots of the mentioned films, I am frightened by the "big brother" and the associated loss of privacy. Today, we almost always communicate to third parties, whether search engines, visited sites or social network operators, an awful lot of information that can be used to extract incredible details about our lives, habits and so on. And they can be easily abused, as in China in their social credit system, which seems very scary to me. And unfortunately it's not sci-fi, but it's here and now, and using it anywhere in the world is "just" a matter of justification. This is associated with the risk of theft of private data or identity by a completely stranger. Although I am glad that the state is gradually digitizing, I have no major illusions about information security. Globally, IT security is often perceived as an unnecessary and expensive luxury, and is basically not addressed until a problem arises. Unfortunately.

Let's leave the IT topic - what about free time?

Ondřej: I recently found a new hobby - I make mechanical keyboards. Otherwise, music or reading to take a break from that computer.

Jan: For me, it's definitely nature and trips. I like to walk in the mountains, in the woods and try to spend as much free time as possible outside the computer and the Internet. On weekends, I prefer to volunteer with the Brontosaurus to take care of valuable natural sites or monuments.

Thank you for the interview,

Ing. Jiří Erlebach (FNUSA-ICRC)