Sereina Riniker, Ph.D. [1]

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Sereina Riniker's lab website [2]

The Eidgenössische Technische Hochschule (ETH) Zurich is one of the world's leading academic research institutions and the intellectual home to nearly 20,000 students and over 500 professors.In summer 2014, Sereina Riniker joined their ranks as their youngest professor, bringing with her a unique experience as a former NIBR postdoctoral scholar.

Sereina started her postdoctoral stay in NIBR Informatics in 2012. Working with mentor Gregory Landrum, she developed an open-source platform for comparing the performance of models that predict the activity of hypothetical drug candidates against disease targets. Dubbed "virtual screening", these computational models assign "molecular fingerprints" that allow one to gauge similarity between molecules, including those that are active or inactive against a disease target. Sereina helped introduce a standardized approach for comparing fingerprinting methods.

This benchmarking platform could be used to test a promising method of combining several virtual screening models into a kind of consensus approach – exceeding the performance of the predictive models applied alone. Furthermore, Sereina developed a novel visualization method to allow investigators to more rapidly and effectively interpret the features of molecules that are important for activity, and she investigated the application of machine-learning methods to data from high-throughput screening.

This work could have a big impact on our ability to zero in on the right drug candidates in disease research.

Sereina says of her experience conducting cheminformatics research at Novartis: "It was a real advantage to be able to focus on the research, surrounded by highly experienced and highly talented scientists, at that stage of my career." "Focus" is the operative word for Sereina. She ended up publishing four first-author papers within just one-and-a- half years.

Doing a postdoc in industry and at NIBR in particular was the right thing for Sereina. "A lot of important methods in cheminformatics came out of industry, so learning about these methods from those who have been using them for years was for me the perfect thing to do." Academia allows Sereina to explore these new approaches in depth in a way that she might not be able to continue to do in industry, and that's why she has moved back to an academic setting. "I'm continuing in the fields I studied for my PhD (molecular dynamics simulations) and my NIBR postdoc". Her research program aims at combining the two fields of computational chemistry in fruitful ways.

So how was the transition from an industrial postdoc at NIBR to an assistant professor at ETH

Zurich? "It was a bit scary at first," she admits. "Suddenly you are responsible for coworkers, you have a budget to take care of, and you need teaching skills. You have to learn very quickly. It's much more than only being a good scientist." For Sereina, the added responsibilities are worth it for the freedom that she now has to explore and discover. She is busy bringing in students and building up her lab while starting her independent research program. Recently, she joined another, rather exclusive group of scientists – the Forbes 2015 "30 under 30" [3] who are among the brightest young scientists, already making discoveries that are changing our world.