Evolutionary molecular dynamics

Methorst, J.

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Curriculum Vitae

Jeroen Methorst was born on the 30$^{\text{th}}$ of August in the city of Apeldoorn, the Netherlands. In 2015, he obtained his bachelor's degree in *Nanobiology* from the Delft University of Technology and the Erasmus University Rotterdam, gaining an interest in the computational aspects of the field.

Continuing his studies in the same field, he performed an internship under the supervision of Dr. Mario Negrello, investigating neuroplasticity using Kuramoto oscillator models. He finalized his master's degree in the lab of Dr. Marie-Eve Aubin-Tam, studying the production of nanoscale-structured composite materials using bacteria under the supervision of Dr. Ewa Spiesz. He graduated in 2018 from the Delft University of Technology and the Erasmus University Rotterdam with his master's degree in *Nanobiology*.

In 2018, Jeroen started his PhD in the Supramolecular and Biomaterials Chemistry group at Leiden University, under the supervision of Prof.dr. Herre Jelger Risselada and Prof.dr. Alexander Kros. Combined interest in machine learning methods and optimization strategies, and molecular dynamics simulations, led to the development of the EVO-MD method described in this thesis. The method is currently seeing application in the development of curvature- and composition-sensing peptides.

Jeroen will continue his research as a postdoc in the group of Prof.dr Herre Jelger Risselada.

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Thanks to Luca for coming up with the name Evo-MD *for our software package and, indirectly, for the title of my thesis.*

I would like to start by thanking my supervisor Jelger. It is a great thing to have a connection with the work and research one is doing, but all that is worth nothing if there is none with the supervisor. Already after my interview (more so the two hour discussion afterwards) I was certain that this would be of no problem. I appreciate your out-of-the-box style of thinking, the "5 steps ahead of the rest" mentality, and encouraging us to take some risk working on what is interesting instead of taking the easy route. I am grateful for the interest you take in your students, especially considering the challenges involved with working in two different countries, and I look forward to continue working with you during my postdoc.

I would also like to thank my promotor Alexander for welcoming us in the SBC group. Even though our theoretical work might seem out of place in this lab-based environment, I have always felt included in the group. Instead of causing division, the different backgrounds and skill sets provided new points of view and insightful discussion in both directions, even leading to several collaborations. In that spirit, thanks to all the members of the SBC group, present and past, for the great social environment, lunchtime discussions, and after-work beer & (usually) pizza. Aimee, Andrea, April, Batuhan, David and David, Dimitris, Dinghao, Don, Elena, Emma, Fred, Gabriela, Hari, Indigo, Isabel, Jasper, Jolinde, Jorn, Joyal, Julia, Lia, Max, Mengjie, Merel, Mertcan, Michele, Michelle, Niek 1, Nol, Oscar, Panagiota, Renzo, Roy, Sabine, Sandeepa, Sofiia, Thomas, Viorica, Winant, Ying, and anyone I might have missed. Thank you all!

A particular thank you goes out to Niek as my closest colleague. With a supervisor in a different country and a field of research very different from the rest of the group, we had to rely on each other during most of our PhD. As it turned out, our different backgrounds, expertise, and occasional viewpoints seemed to complement very well. Thanks for the good times and all the best in San Francisco.

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of post-processing using neural networks, even leading to several publications.

This thesis wouldn't have been possible without all of the collaborators. Many thanks to Dennis for synthesizing the peptides, allowing us to test our predictions, and for all the work with the raft peptides. Loren, Drago, and Jacek, thank you for the collaboration and helping us turn a solely computational idea into a broad analysis of the cholesterol recognition landscape. Of course, Paweł, Christian, Roberto, Partha, and Han are thanked for the work they've put into the project, both experimental and computational.

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Although we have been spread apart over the length of my PhD, working simultaneously in three cities (and two separate countries), it still felt like a group. Thanks to the members of the Risselada group: Laura, Kai, Alireza, Sebastian, Maria, and Max, for the many meetings, discussions, and the great times in Berlin and Dortmund. I'm looking forward to continue working with you all during my postdoc.

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- Jeroen