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Inverse design of curvature-sensing antiviral peptides

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Curriculum Vitae

Niek van Hilten was born in Arnhem on 7 April 1993. He obtained BSc degrees in both *natural sciences* and *molecular life sciences* at Radboud University in Nijmegen. During his studies, he got interested in using computer models to understand biological phenomena. He continued to pursue this interest during the *molecular life sciences* MSc program, still in Nijmegen, with a multidisciplinary internship at the interface between computational modeling, tumor immunology, and bioorthogonal chemistry. For his MSc thesis project, under the supervision of Prof.dr. Peter Kolb at Philipps University in Marburg (Germany), he focused on computational drug discovery and performed a virtual docking screening to find selective small molecule antagonists for the G protein-coupled orexin receptors. Niek graduated *cum laude* in 2017.

In 2018, he started his PhD at Leiden University under the supervision of Prof.dr. Herre Jelger Risselada and Prof.dr. Alexander Kros. Here, as described in this PhD thesis, he performed coarse-grained molecular dynamics simulations of peptide-membrane interactions and embedded those in a evolutionary algorithm framework to design curvature-sensing antiviral peptides.

Next, Niek will continue his scientific career as a post-doc in Prof.dr. Michael Grabe's lab at UCSF in San Francisco.



List of publications

Manuscripts in this thesis

Van Hilten, N.; Stroh, K.S.; Risselada, H.J., Membrane thinning induces sorting of lipids and the amphipathic lipid packing sensor (ALPS) protein motif. *F. Physiol.* **2020**, 11, 250.

Van Hilten, N.; Stroh, K.S.; Risselada, H.J., Efficient quantification of lipid packing defect sensing by amphipathic peptides; comparing Martini 2 & 3 with CHARMM36. *J. Chem. Theory Comput.* **2022**, 18, 7.

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Van Hilten, N.*; Verwei, N.*; Methorst, J; Nase, C.; Bernatavicius, A.; Risselada, H.J., PMIpred: A physics-informed web server for quantitative Protein-Membrane Interaction prediction. *bioRxiv* **2023**

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*These authors contributed equally.

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Methorst, J.; Verwei, N.; Hoffmann, C.; Chodnicki, P.; Sansevrino, R.; Wang, H.; Van Hilten, N.; Aschmann, D.; Kros, A.; Andreas, L.; Czub, J.; Milovanovic, D.; Risselada, H.J., Physics-based inverse design of cholesterol attracting transmembrane helices reveals a paradoxical role of hydrophobic length. *bioRxiv* **2023**

*These authors contributed equally.



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Then, I thank my promotor **Alexander**, who welcomed computer nerds in his purely chemistry-focused research group. Despite our research tools being different, I quickly realized that the scientific interests of our little theoretical cluster and the other PhD students in the SBC group largely overlapped. This meant that I always felt embedded in the department, both socially and in the collaborative projects we ended up working on. In this context, I especially thank my SBC colleagues **Dennis**, **Panagiota**, **Niek C.**, **Alex**, **Roy**, **Winant**, and **Lia**, with whom I most closely collaborated in the last five years.

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