University of Groningen

Numerical simulations of proteins

Ramirez Palacios, Carlos

DOI:
[10.33612/diss.196789826](https://doi.org/10.33612/diss.196789826)

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version
Publisher's PDF, also known as Version of record

Publication date:
2022

[Link to publication in University of Groningen/UMCG research database](#)

Citation for published version (APA):
Ramirez Palacios, C. (2022). *Numerical simulations of proteins: molecular dynamics, docking, and deep learning*. [Thesis fully internal (DIV), University of Groningen]. University of Groningen.
<https://doi.org/10.33612/diss.196789826>

Copyright

Other than for strictly personal use, it is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license (like Creative Commons).

The publication may also be distributed here under the terms of Article 25fa of the Dutch Copyright Act, indicated by the "Taverne" license. More information can be found on the University of Groningen website: <https://www.rug.nl/library/open-access/self-archiving-pure/taverne-amendment>.

Take-down policy

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Downloaded from the University of Groningen/UMCG research database (Pure): <http://www.rug.nl/research/portal>. For technical reasons the number of authors shown on this cover page is limited to 10 maximum.

university of
groningen

Numerical simulations of proteins

Molecular dynamics, docking, and deep learning

PhD thesis

to obtain the degree of PhD at the
University of Groningen
on the authority of the
Rector Magnificus Prof. C. Wijmenga
and in accordance with
the decision by the College of Deans.

This thesis will be defended in public on

Tuesday 11 January 2022 at 12.45 hours

by

Juan Carlos Ramírez Palacios

born on 2 May 1991
in Guerrero, Mexico

Supervisors

Prof. S.J. Marrink
Prof. D.B. Janssen

Assessment Committee

Prof. P.G. Bolhuis
Prof. M.W. Fraaije
Prof. A. Mulholland

The research described in this thesis was carried out at the Groningen Biomolecular Sciences and Biotechnology Institute from the University of Groningen and was financially supported by CONACYT through a doctoral grant.

Cover design by Carlos Ramírez & Francesco Olivari
Printed by Gildeprint

© J.C. Ramírez Palacios, Groningen, the Netherlands, 2021

All rights reserved. No part of this publication may be reproduced or transmitted in any form or by any means, without written permission of the author.

Contents

1) Introduction	7
2) Computational Prediction of ω -Transaminase Specificity by a Combination of Docking and Molecular Dynamics Simulations	35
3) Computational Redesign of an ω -Transaminase from <i>Pseudomonas jessenii</i> for Asymmetric Synthesis of Enantiopure Bulky Amines	73
4) Asymmetric Synthesis of Optically Pure Aliphatic Amines with an Engineered Robust ω -Transaminase	113
5) Unbiased Protein-Ligand Binding with the Coarse-Grained Martini 3 Force Field	131
6) Thermostable D-amino Acid Decarboxylases Derived from <i>Thermotoga maritima</i> Diaminopimelate Decarboxylase	155
7) Protein–Peptide Binding of Adhesin Fragments to a Bacterial Protein <i>N</i> -Glycosyltransferase	177
8) Super High-Throughput Screening of Enzyme Variants by Spectral Graph Convolutional Neural Networks	199
9) Binary Classification of Molecular Dynamics Trajectories using Neural Networks	221
10) Summary	243
11) Samenvatting	247
12) List of publications	251
13) Acknowledgments	252