2021-04-22

COMPUTER SIMULATION AND THEORY OF MACROMOLECULES 2021

Online Workshop – April 23-24, 2021

Workshop Hosts
Helmut Grubmüller, Max Planck Institute for Biophysical Chemistry, Göttingen
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Workshop Website https://www.mpibpc.mpg.de/grubmueller/huenfeld

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ONLINE LIVE PRESENTATIONS (Zoom Webinar)

All participants can join the Zoom Session on April 23 and 24, 2021, starting at 9:00 (CEST)
Topic: Hünfeld 2021: Virtual Workshop on Computer Simulation and Theory of Macromolecules

Please click the link below to join the presentations during both days
https://zoom.us/j/98447506535?pwd=TjFtQm5zTnRTMVF1d2daNUZYK2dTUT09
Passcode: 010818

BREAKS: Virtual Coffee Corner (Wonder) – Open 24/7

Join our virtual coffee corner during the breaks and get in touch with the speakers and other participants for informal discussions! Meet old friends from previous workshops or get to know new people from all over the world! This room will not be chaired and using it is optional.

Please note: It might very well be that running Wonder and Zoom in parallel causes a system conflict (camera and microphone assignment).

https://www.wonder.me/r?id=d3fda194-b2ce-4a6f-9401-6cde4ddaf1bd
Guest Password: Theory2021
Icebreaker Question: What's your research topic?

Poster, Online Workshop, April 23-24, 2021
"COMPUTER SIMULATION AND THEORY OF MACROMOLECULES"

Poster – #294

Optimisation of the Mechanical Stability of Anticalin:CTLA-4 Protein Complex via GoMARTINI Simulations

Presenting author: Adolfo Poma
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A variety of non-immunoglobulin protein scaffolds with potential as alternatives to monoclonal antibodies for nanoparticle-based drug delivery are of high interest for targeting T-cells displaying cytotoxic T-lymphocyte antigen 4 (CTLA-4), a limiting factor is the resistance of the anticalin:CTLA-4 complex to mechanical forces exerted by local shear stress. Here, we used a multi scale approach based on Go-MARTINI approach and single-molecule AFM force spectroscopy (AFM-SMFS) to screen residues along the anticalin backbone and determine the optimal anchor point that maximizes binding strength of the anticalin:CTLA-4 complex. We parametrize the Go-MARTINI approach based on the AFM_SMFS data and the molecular dynamics (MD) simulations using parametrized approach help to explain the mechanisms underlying the geometric dependency of mechanostability in the complex. This process can be related to an unzipping-shear mechanism which is commonly seen in nucleic acids strands. These results suggest that optimization of attachment residue position for therapeutic and diagnostic cargo can provide large improvements without requiring genetic mutation of binding interface residues.