GESELLSCHAFT DEUTSCHER CHEMIKER
ORTSVERBAND SIEGEN

Ankündigung

Am Dienstag, **22. November 2022**, spricht um **16:30 Uhr**
im Hörsaal AR-F 002 des Departments Chemie und Biologie

Prof. Dr. Birgit Strodel

Universität Düsseldorf & Forschungszentrum Jülich

über das Thema

„Computational biochemistry stories of protein aggregation and drug design efforts against Covid-19“

Kaffeerunde ab 16 Uhr im Foyer des Hörsaals AR-F 002, organisiert durch das
JungChemikerForum Siegen

Alle interessierten Kolleginnen und Kollegen, Mitarbeiterinnen und Mitarbeiter und Studierende sind zu diesem Vortrag herzlich eingeladen.
Gäste sind herzlich willkommen.

Der Ortsverbandsvorsitzende
PD Dr. Stephan Bäurle
Tel. 0271 740-4025

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Prof. Dr. Birgit Strodel

Computational biochemistry stories of protein aggregation and drug design efforts against Covid-19

In my group, we work on various computational biochemistry topics ranging from drug development and enzyme design to molecular mechanisms of disease and defense against infection. Common denominators of these topics are that proteins play a central role in each of them, and that we particularly apply all-atom molecular dynamics (MD) simulations with the goal of deciphering the biochemistry and physicochemistry of the processes under study. In my talk, I will focus on two topics, namely protein aggregation involved in the development of neurodegenerative diseases and drug design against Covid-19. Neurodegenerative diseases, such as Alzheimer's and Parkinson's disease feature abnormal protein aggregates that appear in neural tissues. To develop new therapeutic interventions, this self-assembly process must be understood in detail. I will use the example of amyloid-β peptide, aggregation of which is a hallmark of Alzheimer's disease, to show how this aggregation process can be studied using MD simulations, with a particular goal to elucidate the effects of various in vivo components and conditions, such as the presence of cell membranes and the brain extracellular matrix, on the conformational dynamics and aggregation of that peptide. The second topic of my talk will address the drug design problem using Covid-19 as an example. I will show how we combine virtual screening, MD simulations and in vitro assays to identify hit molecules as starting points for lead design.