Theoretical and Computational Biophysics Group

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Title: "Molecular Simulations in Times of COVID-19"
Thursday, October 22, 2020
11:00 AM – 12:00 PM
Please click the link below to join the webinar:
https://illinois.zoom.us/j/82104292473?pwd=S1RCb3ZuYlBIZWROb1p3eG95aUdVdz09
Password: 412764

ABSTRACT:
We use molecular dynamics (MD) simulations to study key molecular processes of the SARS-CoV-2 virus. We concentrate on the structure of the spike (S) protein at the viral surface, its interactions with the host cell, and on viral modulation of the host immune response. In molecular dynamics (MD) simulations of full-length S with a palmitoylated transmembrane domain and a fully glycosylated ectodomain, we identified three hinges in the stalk connecting the S head to the viral membrane. Hinge flexibility and glycosylation have been confirmed by high-resolution cry-electron tomography (Turonova, Sikora, Schürmann et al., Science 2020). We are now using the detailed structural and dynamic models for a computational antibody epitope scan (Sikora et al., biorxiv). In addition, we study the interactions of S with the host-cell receptor ACE2 (Mehdipour, Hummer, biorxiv). In MD simulations of the SARS-CoV-2 papain-like protease PLpro, MD simulations provided detailed insight in its function as immunomodulator by suppressing the host interferon (IFN) and NF-κB pathways through preferential cleavage of ISG15 (Shin et al., Nature 2020). Overall, MD simulations help us to uncover some remarkable biology associated with viral infection and, as we hope, guide our fight against COVID-19.

Acknowledgments. Our special thanks go to Martin Beck and Beata Turonova plus team (MPIBP and EMBL) for the electron tomography, to Jacomine Krijnse Locker and Christoph Schürmann plus team (Paul Ehrlich Institute) for the virus purification, and to Donghyuk Shin and Ivan Dikic plus team (Goethe University and MPIBP) for the structural and mechanistic studies of PLpro.

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