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VABILO NA PREGLOV KOLOKVIJ / INVITATION TO THE PREGL COLLOQUIUM

Prof. Bert de Groot, Ph.D.

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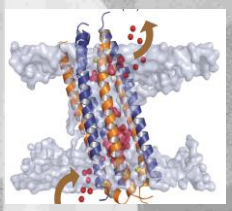
Četrtek, Thursday, 8. 5. 2014, ob / at 13:00

Velika predavalnica Kemijskega inštituta / Lecture Hall at the National Institute of Chemistry; Hajdrihova 19, Ljubljana

Molecular dynamics of inhibition, permeation and recognition

Can we design specific membrane channel inhibitors? What is the antimicrobial mechanism of the human antibiotic dermcidin? What are the molecular determinants of channel permeation and gating? What is the molecular basis of protein-protein recognition, and can we alter protein binding affinity by computational design? These are some of the questions that are addressed at the atomic level by molecular dynamics simulations.



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[2] Ulrich Zachariae, Robert Schneider, Rodolfo Briones, Zrinka Gattin, Jean-Philippe Demers, Karin Giller, Elke Maier, Markus Zweckstetter, Christian Griesinger, Stefan Becker, Roland Benz, Bert L. de Groot, and Adam Lange. *Beta-barrel mobility underlies closure of the voltage-dependent anion channel.* Structure**.** 20:1540-1549 (2012).
[3] Chen Song, Conrad Weichbrodt, Evgeniy S. Salnikov, Marek Dynowski, Björn O. Forsberg, Burkhard Bechinger, Claudia Steinem, Bert L. de Groot, Ulrich Zachariae, and Kornelius Zeth.*Crystal structure and functional mechanism of a human antimicrobial membrane channel.* Proc. Nat. Acad. Sci. 110: 4586-4591 (2013).
[4] Carsten Kutzner, Helmut Grubmüller, Bert L. de Groot, Ulrich Zachariae. *Computational Electrophysiology: The Molecular Dynamics of Ion Channel Permeation and Selectivity in Atomistic Detail.* Biophys. J. 101: 809-817 (2011).
[5] Jan-Henning Peters and Bert L. de Groot. *Ubiquitin dynamics in complexes reveal molecular recognition mechanisms beyond induced fit and conformational selection.* PLoS Comp. Biol. 8: e1002704 (2012).

Vljudno vabljeni! / Kindly invited!

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