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Molecular dynamics of prototype foamy virus protease flap region, N- and C-termini in aqueous solution

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Molecular dynamics trajectories are Cartesian coordinates produced by recording of dynamical changes over time representing the positions of each atom along a series of small time step. Here, we implemented atomistic molecular dynamics simulations of prototype foamy virus (PFV) protease monomer to investigate the conformational changes of the flap region, N- and C-termini in aqueous solution. The PFV protease monomer undergoes some changes of secondary structure but remains stable during 10 ns simulation time. In particular, the flap region and the N- and C-termini turned out to be highly flexible. Nevertheless, retroviral protease dimerization process occurs through the anti-parallel β -sheet, which is absent in the PFV protease. Although the overall folds of β -sheets and α -helices are remained quite similar and stable, the PFV protease dimerization mechanism reveals significant differences in the dimerization interface relative to other retroviral proteases, such as HIV protease. Therefore, PFV protease dimerization event might be mediated through the additional viral or cellular cofactors. Finally, the results provide a model for the flap region, N- and C-termini overall dynamics that is considered to be important for regulation of the enzyme function.

Biography

Dr. Sergey Shityakov M.D Ph.D is a virologist from the Institute for Virology and Immunobiology (VIM) University of Würzburg in Germany. He has a wide experience in applied experimental and theoretical research ranging from basic virology to computational biochemistry. He is recognized for conducting research on retroviruses such as human immunodeficiency viruses (HIV) and prototype foamy viruses (PFV) to elucidate the mechanism of their nuclear import. His several papers regarding to retroviral pathogenesis and functional morphology have been published in various international peer-reviewed scientific journals. He is currently working at the University of Würzburg in the department of bioinformatics. He holds a membership of the Euroscience Association.