Tutorial: Using the UNRES server and the standalone UNRES package in SAXS-data-assisted modeling of protein structure

Agnieszka S. Karczyńska,[1] Emilia A. Lubecka,[2] Cezary Czaplewski[1] and Adam Liwo[1]

[1]Faculty of Chemistry, University of Gdansk, Wita Stwosza 63, 80-308 Gdańsk, Poland

[2]Institute of Informatics, Faculty of Mathematics, Physics, and Informatics, Wita Stwosza 57, 80-308 Gdańsk, Poland

adam.liwo@ug.edu.pl

The UNRES package (www.unres.pl), which is also available as UNRES server (http://unres-server.chem.ug.edu.pl) [1] enables the users to carry out coarse-grained molecular dynamics simulations of protein structure with the UNRES force field [2]. Small angle x-ray scattering (SAXS) data can be entered in the form of distance distribution to restrain the simulations, the restraint function being defined as a maximum-likelihood term to keep the calculated distance distribution close to the experimental distribution [3]. In this tutorial we will illustrate with selected examples how to carry out SAXS-restrained simulations with the UNRES server. Those interested will also be given the opportunity to learn how to install UNRES and run it on their systems. On-site assistance will be provided to participants interested in getting help to run SAXS-assisted UNRES on the proteins they are working on.

[1] C. Czaplewski, A. Karczyńska, A.K. Sieradzan, A. Liwo. *Nucleic Acids Research*, 2018, 46, W304–W309.

[2] A. Liwo, M. Baranowski, C. Czaplewski, E. Gołaś, Y. He, D. Jagieła, P. Krupa, M. Maciejczyk, M. Makowski, M.A Mozolewska, A. Niadzvedtski, S. Ołdziej, H.A. Scheraga, A.K. Sieradzan, R. Ślusarz, T. Wirecki, Y. Yin, B. Zaborowski. *J. Molec. Model.*, 2014, 20, 1-15.

[3] A.S. Karczyńska, M.A. Mozolewska, P. Krupa, A. Giełdoń, A. Liwo, C. Czaplewski. *Proteins: Struct. Func. Bioinfo.*, 2018, 86 (S1), 228-239.