MS10-P2 Transferable aspherical atom model refinement of protein and DNA structures against ultra-high-resolution X-ray data

Maura Malinska[1], Zbigniew Dauter[1]

1. Synchrotron Radiation Research Section, MCL, National Cancer Institute, Argonne National Laboratory, Argonne, IL 60439, USA

email: mmalinska@anl.gov

In contrast to the independent atom model (IAM), in which all atoms are assumed to be spherical and neutral, transferable aspherical atom model (TAAM) takes into account charge transfer and deformation of the valance charge density resulting from the chemical bond formation, the presence of lone electron pairs, or intra- and intermolecular interactions. Both models can be used for refinement of small and large molecules e.g. proteins and nucleic acids, against ultra-high-resolution X-ray diffraction data. The University at Buffalo theoretical databank of aspherical pseudoatoms has been tested in the refinement of the tripeptide Phe-Val-Phe, Z-DNA hexamer duplex, Z-DNA dodecamer and aldose reductase. Application of the TAAM to these data improves quality of density maps and visibility of hydrogen atoms. It also slightly lowers the conventional R factor, improves the atomic displacement parameters and the results of the Hirshfeld rigid-bond test. Additional advantage is that the transferred charge density permits to estimate Coulombic interaction energy and electrostatic potential.

Keywords: structure, precision and accuracy, interaction

MS10-P3 Purification, structural characterization and homology modeling of a novel neurotoxic peptide (Acra3) from the scorpion Androctonus crassicauda

Suheyla Ozbey[1], Damla Koçak[1], Filiz Betul Kaynak[1], Figen Çalışkan[2]

1. Department of Engineering Physics, Hacettepe University, 06800 Beytepe, Ankara, Turkey
2. Department of Biology, Faculty of Science and Art, Eskisehir Osmangazi University, 26480 Eskisehir, Turkey

email: sozbey@hacettepe.edu.tr

Androctonus crassicauda is one of the Southeastern Anatolia scorpions of Turkey with ethnomedical and toxicological importance. Information on the biochemistry, pharmacology, active principles and mechanism of action of the venom is crucial for the development of specific antivenoms. The venom group in the Biology Department of Eskisehir Osmangazi University is focused at the characterization of the main components of this scorpion venom, due to the fact that very little is known thus far on this species.

The isolation of neurotoxic peptide Acra3 by chromatographic separations (HPLC and TSK-gel sulfopropyl) and its chemical and functional characterization were also performed and recently reported (Caliskan et al. 2012, Peptides 37: 106–112). Acra3 is a 7620 Da molecular weight peptide, with 66 amino acid residues and has eight cysteine residues, crosslinked by four disulfide bridges.

We have currently carried out the structural characterization of Acra3 peptide by using the small angle x-ray solution scattering. From the small angle scattering data overall structural parameters of the protein e.g. molecular radius of gyration (Rg), maximum particle diameter (Dmax) were derived. .

Furthermore, three-dimensional structure modeling of Acra3 was also predicted by amino acid sequence alignment and then homology modeling by using FASTA and CLUSTALW EBI and Swiss Model servers. These models will be used as the starting point for nanosecond-duration molecular dynamics simulations.

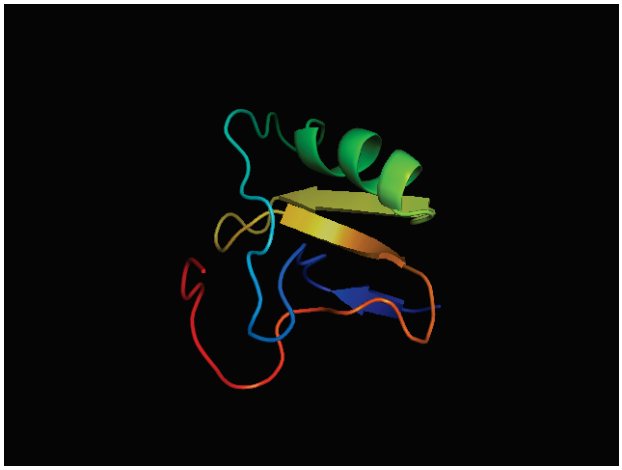

Figure 1. Homology structure of Acra3

Keywords: scorpion peptide, Acra3, Androctonus Crassicauda, homology modeling