УДК: 61:615.1(043.2)
ББК: 5:52.8
ISBN: 978-985-21-0532-3

Nadim Mousa

CALCIUM (II) CATIONS BINDING BY PROTEINS OF *STAPHYLOCOCCUS AUREUS*

Scientific Supervisor Ph.D., associate professor Vladislav Khrustalev
Department of General Chemistry
Belarusian State Medical University, Minsk

Relevance. It has been widely accepted that Calcium (II) metalloenzymes adopt a helix-loop-helix structural domain (EF hand). Calcium binding proteins such as Parvalbumin, Calmodulin-kinases, and Troponin C play a role in a variety of physiological processes, including cell-cycle regulation, second messenger production and muscle contraction. Applying computational algorithms aids in the investigation of amino acid interactions and secondary structure of Ca^{2+} metalloenzymes. Discovering if Ca^{2+} metalloenzymes only present in EF hand structural domain, or can adopt other forms should contribute into better understanding of the biochemical function of these proteins.

Purpose of the study: analyzing the structural motif and amino acid content of Ca^{2+} metalloenzymes.

Methods and procedures. The set of nonhomologous proteins (35) which coordinate bonds with Ca^{2+} in *Staphylococcus aureus* has been selected from the Protein Data Base. The enzymes were run on the protein ligand interaction profiler (PLIP) to determine amino acid interactions with Ca^{2+} cations. Secondary structure database with the results of description of secondary structure by DSSP algorithm and the results of 5AI algorithm of chemres.bsmu.by provided us with the motif and amino acid contents of the proteins, which were compared to the PLIP results. T-values were calculated to analyze the significance of these results.

Results and discussion. Secondary structure motifs around all amino acid residues that bind Ca^{2+} cations have been studied. Residues making coordination bonds with Ca^{2+} are overrepresented mainly in the region between two β strands. They are also highly frequent in three β strands motif, but they are not overrepresented in that motif compared with the control. Amino acid residues from outer spheres of Ca^{2+} complexes seem to be overrepresented in random coil between α helix and β strand relatively to the control. Indeed, binding residues are significantly overrepresented in well described Ca^{2+} motif (a loop between two α helices), but not that much. There are differences in amino acid content between PLIP and 5AI results. Overrepresentation of Asp, Glu, Gly, His, and Ser was found in PLIP results. While 5AI results showed overrepresentation of Asp, His, Ser, Ala, Cys, and Asn.

Conclusion. With such a small dataset, it is hard to obtain reliable and conclusive results. The dataset was found to contain 30% beta-structural, 19% alpha-structural proteins; while 51% of proteins had mixed domains. These results show the ability of Ca^{2+} metalloenzymes to bind Ca^{2+} by beta-coil-beta structural motifs; although more research has to be conducted with a bigger dataset containing more alpha-helical proteins for more definite results.