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Molecular Modeling of Extremophilic-related Proteins of *Deinococcus radiodurans*

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The Deinococcaceae group comprises some of the robust known extremophilic bacteria. Attempts to explain mechanisms of *Deinococcus radiodurans* against simultaneous stresses, have especially focused its responses against extreme doses of gamma radiation. *D. radiodurans* has many defensive mechanisms, and transcriptomes already made in response to gamma radiation and desiccation revealed that some genes were transcribed to proteins of undefined functions, while others have never been expressed. Therefore, it is expected that such genes with obscure function can code for novel resistance proteins to extreme conditions and help comprehension on these extremophilic functions. Our research aims to identify and perform function prediction for hypothetical, unique proteins of *D. radiodurans*, without similarity to any other known protein. We selected a group of proteins, expressed in *D. radiodurans* after gamma radiation, which hypothetical functions were predicted by the best scores after Psi-BLAST alignments and CD-search. Information about the proteins was gathered through alignments against Uniprot and PDB databases. Using molecular modeling tools as I-TASSER and SWISS MODEL, we generated 3D models for all proteins and they were initially evaluated by Ramachandran's Plot and RMSD. The best models were then submitted to structural classification on SCOP and CATH servers. That way, we were able to speculate on the function of some candidates, and produce other models if structural and sequential annotation disagree. Our results reveal promising candidates for future biotechnological approaches. DR_2441 is quite similar to N-acetyl transferases from extremophilic bacteria, which probably accounts for a detox mechanism by antioxidant bacillithiol. DR_1370 was also found as an important lipid anchor lipoprotein belonging to the Lol family. Other proteins seem to bind to nucleic acids, acting on metabolic regulation under severe conditions. This particular resistance toolbox was defined as the "Black Box Genome of *D. radiodurans*".

Palavras-chave: *Deinococcus*; Extremophile; Protein
Patrocínio: CNPQ