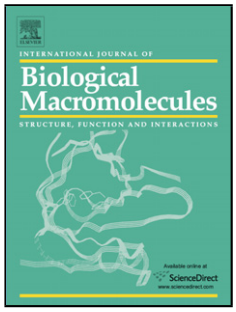

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Anion–π interactions in active centers of superoxide dismutases

Vesna R. Ribić[a], Srđan Đ. Stojanović[b], Mario V. Zlatović[c,*]

* Corresponding author.
E-mail address: mario@chem.bg.ac.rs

[a] Institute for Multidisciplinary Research, Department of Materials Science, University of Belgrade, Belgrade, Serbia

[b] ICTM - Department of Chemistry, University of Belgrade, Belgrade, Serbia

[c] Center for Computational Chemistry and Bioinformatics, Faculty of Chemistry, University of Belgrade, Belgrade, Serbia

Abstract

We investigated 1060 possible anion–π interactions in a data set of 41 superoxide dismutase active centers. Our observations indicate that majority of the aromatic residues are capable to form anion–π interactions, mainly by long-range contacts, and that there is preference of Trp over other aromatic residues in these interactions. Furthermore, 68% of total predicted interactions in the dataset are multiple anion–π interactions. Anion–π interactions are distance and orientation dependent. We analyzed the energy contribution resulting from anion–π interactions using *ab initio* calculations. The results showed that, while most of their interaction energies lay in the range from –0 to –4 kcal mol^{-1}, those energies can be up to –9 kcal mol^{-1} and about 34% of interactions were found to be repulsive. Majority of the suggested anion–π interacting residues in ternary complexes are metal-assisted. Stabilization centers for these proteins showed that all the six residues found in predicted anion–π interactions are important in locating one or more of such centers. The anion–π interacting residues in these proteins were found to be highly conserved. We hope that these studies might contribute useful information regarding structural stability and its interaction in future designs of novel metalloproteins.

Keywords

Anion–π interactions · Superoxide dismutase · Proteins · Active centers · Interaction energy