ISSN 2334-6590
UDK 57 (051)

Biologia Serbica

Book of Abstracts
Belgrade BioInformatics Conference 2018

Volume 40 - No. 1
(Special Edition)
2018

BELBI 2018

Department of Biology and Ecology
Faculty of Sciences
University of Novi Sad

P7

Binding of metal ions and water molecules to nucleic bases

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Abstract:
Hydrogen bond interactions between nucleic bases and water have been analyzed by surveying Protein Data Bank (PDB) and quantum chemical calculations, for the noncoordinated and coordinated water molecule. Python home-made script was used for the PDB search and Gaussian09 program was used for the calculations of interaction energy at MP2/def2-QZVP level on model systems. The results from PDB survey and from the calculations are in agreement: hydrogen bonds are shorter and stronger when water is bonded to a metal ion.

The PDB search data show that metal ions prefer to bind nucleic acids through water than directly by coordination. Mg, Sr and Na are the most common metals to interact with nucleic bases through water molecule. It was shown that 19.2 % of metal-nucleic interactions are double hydrogen bonds and Mg and Sr are the most prone to form multiple hydrogen bonds with nucleic bases.

The calculated interaction energies for [Mg(H2O)6]2+ complex are in the range of (-12.94 to -49.96) kcal/mol, and for [Na(H2O)6]+ complex in the range of (-6.66 kcal/mol to -19.63) kcal/mol, while the interaction energies for noncoordinated water are (-4.63 to -8.93) kcal/mol. These calculated values for water-nucleic base hydrogen bonds are comparable to the strength of hydrogen bonds between nucleic bases (-5 to -47 kcal/mol) calculated previously, so these results may be relevant to understand the role of water molecules and metal ions in the process of replication and stabilization of nucleic acids and also toxicity.

Keywords:
nucleic base, metal, hydrogen bond, Protein Data Bank

This work has been funded by MESTD, Republic of Serbia (project 172065).

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