The first hydration layer around biomolecules is site-specific

L. Biedermannová, B. Schneider

Institute of Biotechnology, Czech Academy of Sciences, Prumyslova 595, Vestec, 252 50, Czech Republic

Lada.Biedermannova@ibt.cas.cz

Proteins and nucleic acids evolved in the aqueous environment, and water is therefore deeply interrelated with both biomolecular structure and function. The first layer of water molecules around the biomolecular surface - the hydration shell - has properties different from the bulk water [1]. The dynamics of these water molecules is significantly reduced, and the shell mostly consists of ordered (localized) water molecules. However, the first shell water molecules do not have an ice-like structural properties. These ordered water molecules play significant role in recognition and binding of ligands.

In our work, we utilize crystallographic data to compile the average hydration patterns around biomolecules. Firstly, we investigated hydration of DNA building blocks [2, 3], and later hydration of amino acids in proteins as a function of their rotameric state and the secondary structure [4, 5]. Recently, we analyzed hydration of DNA dinucleotides as a function of their conformation and sequence [6]. Here, we present an overview of these results as well as the methodology we used to obtain the data and the potential application of the results.

[1] Biedermannová L. & Schneider B. (2016). *Biochim. Biophys. Acta – Gen. Subj.* **1860**, 1821.

[2] Schneider B. & Berman H. M (1995). *Biophys. J.* **69**, 2661 .

[3] Schneider B., Patel K. & Berman H. M. (1998). *Biophys. J.* **75**, 2422.

[4] Biedermannová L. & Schneider B. (2015). *Acta Cryst.* **D71**, 2192.

[5] Černý J., Schneider B. & Biedermannová L. (2017). *Phys. Chem. Chem. Phys.* **19**, 17094.

[6] Biedermannová L. *et al.*, (2021). *In preparation*.

Keywords: hydration; proteins; nucleic acids; structural biology; X-ray crystallography.