

MS05-1-3 Prediction of DNA hydration based on data mining of crystallographic structures
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Abstract

Water plays an important role in stabilizing DNA structure and in mediating its interactions. In our work, we utilize crystallographic data to compile the average hydration patterns around biomolecules - proteins [1,2,3] and nucleic acids [4,5,6]. Recently, we investigated hydration of DNA as a function of its conformation and sequence. We analyzed hydration of DNA dinucleotides from an ensemble of 2,727 non-redundant DNA chains containing 41,853 dinucleotides and 316,265 associated first-shell water molecules [6].

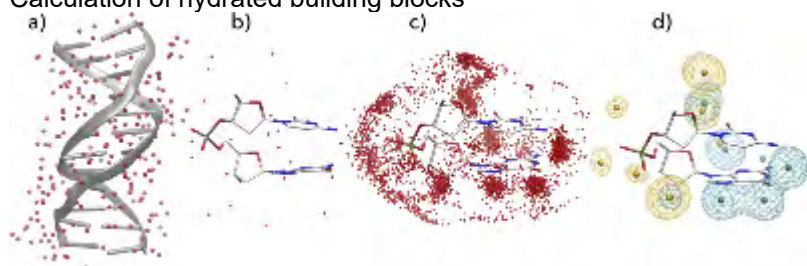
The dinucleotides were classified into categories based on their 16 sequences and the previously determined structural classes, so called nucleotide conformers (NtCs). The construction of hydrated dinucleotide building blocks allowed dinucleotide hydration to be calculated as probability of water density distributions (Figure 1). Peaks in the water densities - Hydration Sites (HSs) - uncovered the interplay between the base and the sugar-phosphate hydration in the context of sequence and structure.

Here, we present the overview of these results and the potential application of the the hydrated building blocks for the prediction of DNA hydration (Figure 2). The data for the hydrated building blocks and the predictions are available for browsing and visualization at the website watlas.datmos.org/watna.

References

- [1] Biedermannová L. & Schneider B.: Structure of the ordered hydration of amino acids in proteins: analysis of crystal structures. *Acta Crystallographica D* 71: 2192-2202 (2015). [2] Černý J., Schneider B. & Biedermannová L.: WatAA: Atlas of Protein Hydration. Exploring synergies between data mining and ab initio calculations. *Phys. Chem. Chem. Phys.* 19, 17094 (2017). [3] Biedermannová L. & Schneider B.: Hydration of proteins and nucleic acids: Advances in experiment and theory. A review. *Biochimica et Biophysica Acta - General Subjects* 1860: 1821-1835 (2016). [4] Schneider B. & Berman H.M.: Hydration of the DNA Bases Is Local. *Biophysical J.* 69: 2661-2669 (1995). [5] Schneider B., Patel K. & Berman H.M.: Hydration of the Phosphate Group in Double-Helical DNA. *Biophysical J.* 75: 2422-2434 (1998). [6] Biedermannová L. et al., *Acta Cryst D*, under consideration (2022).

Calculation of hydrated building blocks



Predicted (yellow and cyan) vs crystal water (red)

