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Hydration dynamics of nucleic acids: molecular origin of the heterogeneity and sequence dependence

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ABSTRACT

The displacement of water molecules from DNA or RNA hydration shells is a key step in important biological processes such as drug binding to DNA, DNA compaction around histones, or the formation of RNA-protein complexes during gene expression. Hence, understanding the properties of nucleic acid hydration shells is a first important step to gain a molecular-level understanding of these processes.

Building on our previous work on a model DNA dodecamer [1], we extend our study to various DNA and RNA sequences, where we obtain from molecular dynamics simulations a site-resolved map of water reorientation dynamics. We rationalize the heterogeneity in the hydration dynamics using the jump model for water reorientation, and examine how hydration shell dynamics correlates with parameters (e.g. groove width and depth) commonly used to describe the DNA double helix structure. We show key differences between the hydration dynamics of analogous DNA and RNA sequences and investigate their molecular origin.

REFERENCES

[1] E. Duboué-Dijon, A.C. Fogarty, J. T. Hynes, D. Laage, J. Am. Chem. Soc., **138**, 7610-7620 (2016)