

# The first hydration layer around biomolecules is site-specific

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*Computational Approaches to RNA Structure and Function*

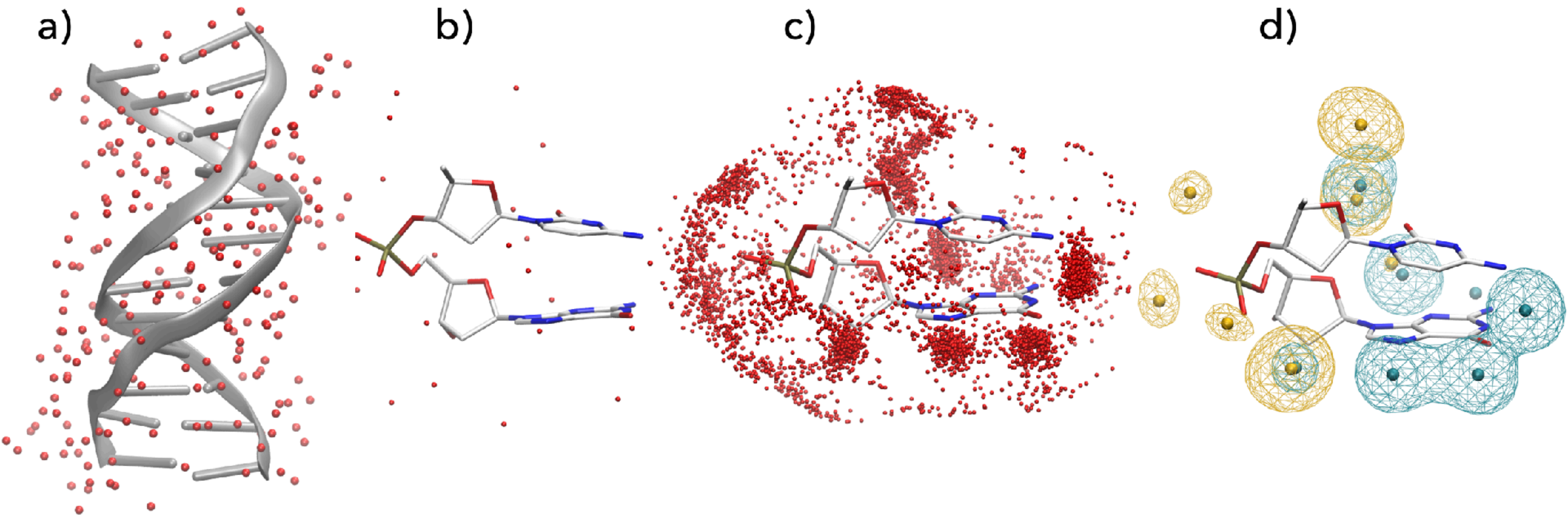
2024-07-26



# Background

- Proteins and nucleic acids evolved in the aqueous environment.
- The 1st hydration shell has properties different from the bulk water.
  - 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).
- Water dynamics in the hydration shell is reduced compared to the bulk.
  - Bohdan Schneider, Jean-Christophe Gelly, Alexandre G. de Brevern & Jiří Černý: Local dynamics of proteins and DNA evaluated from crystallographic B factors. *Acta Cryst. D70*: 2413–2419 (2014).
- The first hydration shell consists of mostly ordered (localized) water molecules.
- Proteins:
  - Biedermannová L. & Schneider B.: Structure of the ordered hydration of amino acids in proteins: analysis of crystal structures. *Acta Cryst D71*: 2192-2202 (2015).
- DNA:
  - Lada Biedermannová, Jiří Černý, Michal Malý, Michaela Nekardová & Bohdan Schneider: Knowledge-based prediction of DNA hydration using hydrated dinucleotides as building blocks. *Acta Cryst. D78*: 1032–1045 (2022).
- The release of the ordered hydration water is entropically favorable, enthalpically neutral.

# The Protocol

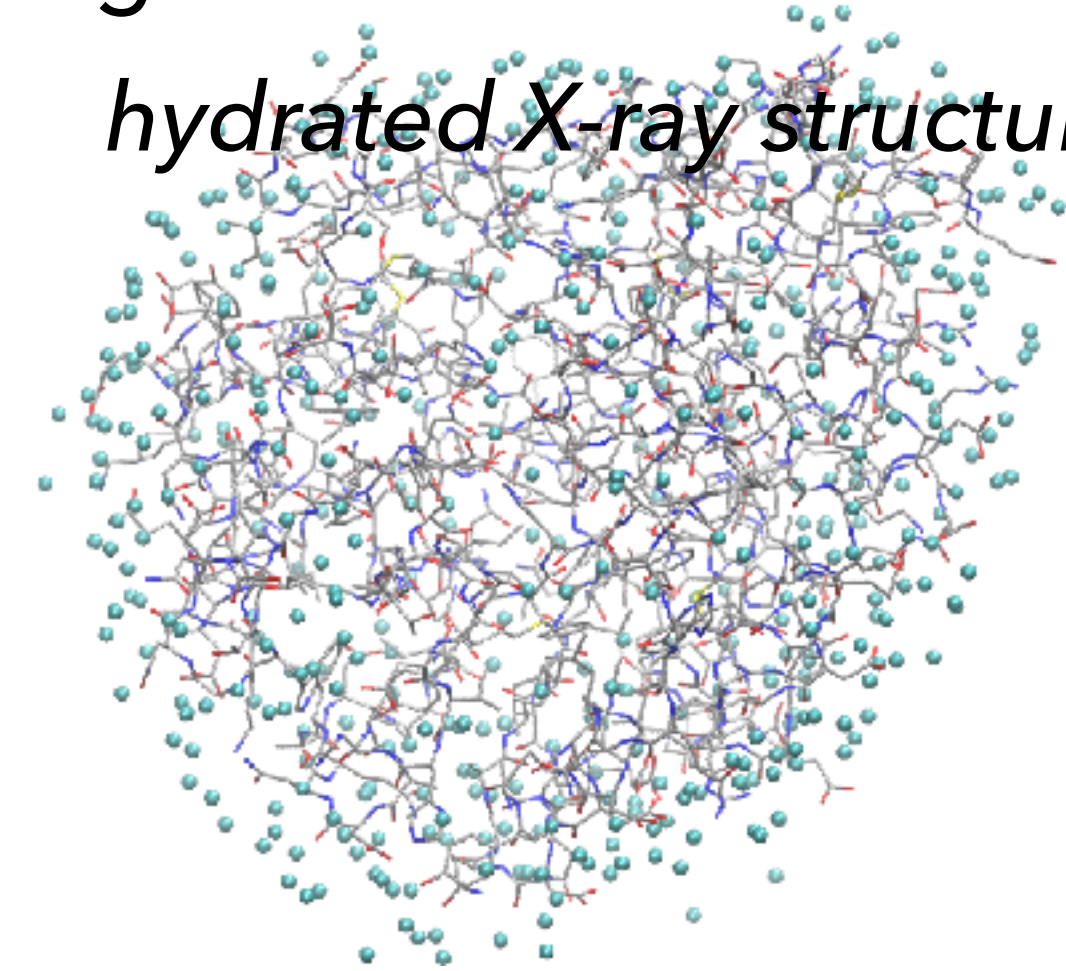


RCSB **PDB**  
PROTEIN DATA BANK

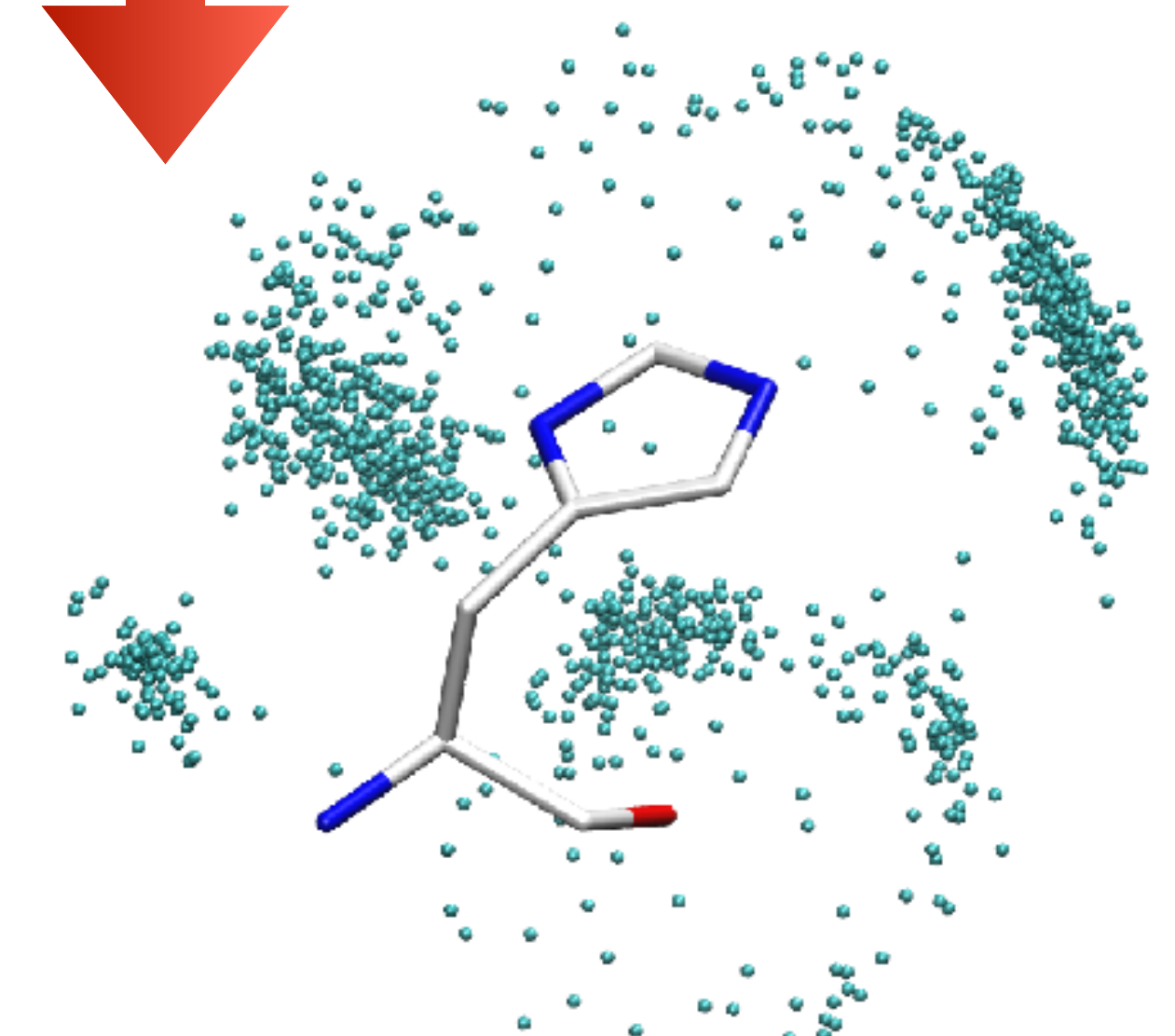
*Database search for suitable  
biomolecular X-ray structures*

Select structures

*Large number of well-resolved,  
hydrated X-ray structures*

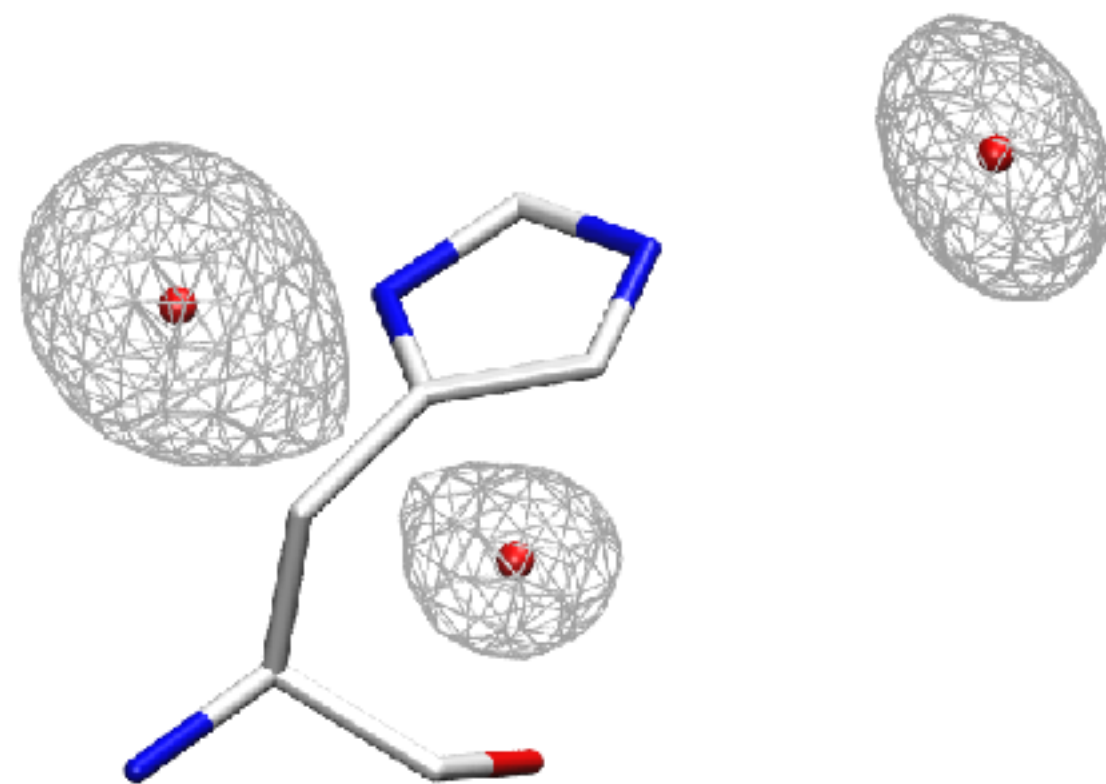


Extract hydrated fragments



*Relevant water molecules  
added to a reference fragment*

Fourier Averaging



*Hydration sites identified  
as maxima in water density map*

# The Key Point of Our Hydration Analysis

- You rely on sensibly selected fragment
- When the fragment has conformational freedom, you must have well clustered conformers
  - rotamers for amino acids
  - NtC dinucleotide classes for DNA and RNA

# To Be Finished

- Interpretation of RNA hydration patterns
- RNA hydration to water

# The website

- 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).

