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Binding of metal ions and water molecules to nucleic bases

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Introduction

Hydrogen bonds of coordinated water are much stronger than those between noncoordinated water molecules [1,2]. The nucleic base – coordinated water interactions are applied in heavy metal ion detection [3] as artificial short single-stranded DNA or RNA sequences can fold into specific secondary and tertiary structures on binding to certain heavy metal targets with extremely high specificity.

Results

- *Both PDB search and calculations revealed shorter hydrogen bonds with coordinated water, with the acceptor-donor distance in the range of 2.7–2.8 Å independently of metal type, in contrast to the noncoordinated water in the range of 2.9–3.1 Å.*
- *A number of interactions found in PDB are of type nucleic base - hydrated metal – protein, which points out that hydrated metal ions can intermediate protein-DNA contacts*
- *The results of the calculations show that the hydrogen bond interactions for doubly charged $[Mg(H_2O)_6]^{2+}$ complex (-12.94 to -49.96 kcal/mol) and for singly charged $[Na(H_2O)_6]^{+}$ complex (-6.66 kcal/mol to -19.63 kcal/mol) are stronger than for noncoordinated water (from -4.63 to -8.93 kcal/mol)*

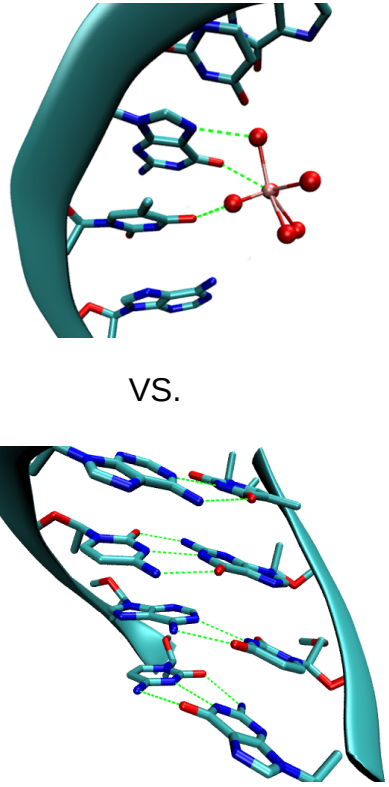

Figure 1. Interactions of nucleic bases with water coordinated to Mg^{2+} (up) and with other nucleic bases in DNA structure (down). Hydrogen bonds represented in green dashed lines. PDB id: 5E36.

Methodology

- *The hydrogen bond interactions of nucleic bases with noncoordinated and coordinated water molecule were studied by analysing geometry of 2402 Protein Data Bank [4] crystallographic structures. Python homemade script was used for the PDB search*
- *MP2/def2-QZVP quantum chemical calculations implemented in the ORCA software [5]*

Conclusion

- *The calculated values for hydrogen bond interactions are comparable to the strength of hydrogen bonds between nucleic bases which span from -5 to -47 kcal/mol [6] (Figure 1)*
- *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 as well as possible toxicity*

References

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