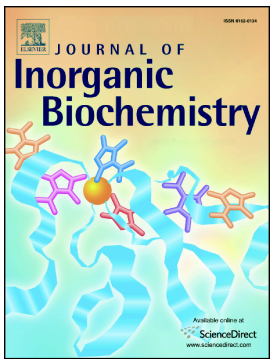

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PII: S0162-0134(17)30470-1
DOI: doi:10.1016/j.jinorgbio.2017.10.010
Reference: JIB 10355

To appear in: *Journal of Inorganic Biochemistry*

Received date: 30 June 2017
Revised date: 19 October 2017
Accepted date: 25 October 2017

Please cite this article as: Riccardo Bonsignore, Fabrizia Russo, Alessio Terenzi, Angelo Spinello, Antonino Lauria, Giuseppe Gennaro, Anna Maria Almerico, Bernhard K. Keppler, Giampaolo Barone , The interaction of Schiff Base complexes of nickel(II) and zinc(II) with duplex and G-quadruplex DNA. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Jib(2017), doi:10.1016/j.jinorgbio.2017.10.010

The interaction of Schiff Base complexes of nickel(II) and zinc(II) with duplex and G-quadruplex DNA

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Abstract

The duplex and G-quadruplex DNA-binding of six nickel(II) and zinc(II) complexes of three salphen-like ligands (salphen=N,N'-bis-salicylidene-1,2-phenylenediaminato) was investigated by UV-visible absorption and circular dichroism spectroscopy. The results obtained, in particular the values of the DNA-binding constants, K_b, point out that the nickel(II) complexes show a higher affinity towards both duplex and G-quadruplex DNA, compared to the analogous zinc(II) complexes. Interestingly, the zinc(II) complexes possess high selectivity toward G-quadruplex DNA, being negligible their binding with duplex DNA. Molecular dynamics (MD) simulations provided atomistic models for the interpretation of the binding of the zinc(II) complexes with G-quadruplex DNA, allowing a structural comparison of the three salphen-like ligands, due to the presence of different substituents (H, F, CF_3) on the position 4 of the phenyl ring on the N,N' bridge.

Keywords: Binding Constant; Computational Chemistry; DNA; G-quadruplex; Nickel; Zinc