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findings highlight these NEET proteins as promising mitochondrial targets for cancer therapy.
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DNA recognition of Copper complexes using metadynamics simulations and hyperfine coupling calculations

The ability of many organic and coordination compounds to bind to DNA and/or damage cellular structures has been largely exploited in anticancer research. Identifying DNA recognition mechanisms have thus important impact on the chemical biology of gene expression and the development of new drugs and therapies. Previous studies on copper(II) complexes with oxindole-Schi® base ligands have shown their potential anti-tumor activity towards di®erent cells, inducing apoptosis through a preferential attack to DNA and/or mitochondria[1]. The binding mechanism of the organic like as Furamidine (1) and copper(II) complexes [Cu(isaepy)2]2+ (2) and [Cu(isaenim)]2+ (3) and their modulation at DNA is investigated through theoretical studies. Here we adopted a multi-scale procedure to simulate this large system using classical molecular dynamics and metadynamics. The main purpose of this work is to investigate its modes and binding mechanisms of the organic compound (1) and metal complexes (2) and (3) in DNA using classical metadynamics simulations. Free energies of binding are investigated by metadynamics enhanced sampling methods[2]. Hybrid Car-Parrinello/Molecular Mechanics calculations were applied to parameterize the copper(II) complexes by using the force matching approach. We acknowledge support from CAPES, INEO and CNPQ.