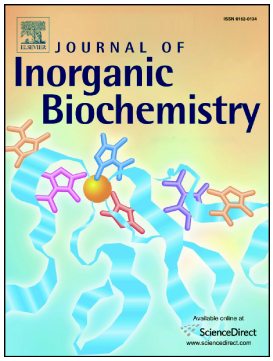

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Synthesis, Crystal Structure and Hydrolysis Activity of a Novel Heterobinuclear Cobalt(III) Sodium(I) Schiff Base Complex

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Abstract A novel heterobinuclear complex $[CoNa(C_{15}H_{10}NO_4F)_2(CH_3OH)]_2$ with Schiff base ($C_{15}H_{10}NO_4F$: 2-amino-4-fluorobenzoic acid—3-methoxysalicylaldehyde) was synthesized and characterized by IR and ^1H NMR spectroscopy, elemental analysis and single crystal X-ray diffraction. X-ray crystallography reveals that the cobalt atom is six-coordinated by two nitrogen atoms from -C=N-, two carboxylate oxygen atoms and two hydroxyl oxygen atoms in different ligands, while the sodium atom is seven-coordinated by two methoxy oxygen atoms, two hydroxyl oxygen atoms in different ligands, two oxygen atoms in the same carboxylate and one oxygen atom of solvent methanol. The reaction results of the complex with the *p*-nitrophenylphosphate (pNPP) and the adenosine monophosphate (AMP) reveal that the complex can hydrolyze phosphoester bonds. Then the DNA-hydrolysis activity is studied experimentally and theoretically, indicating that the complex can effectively hydrolyze the pBR322 supercoiled plasmid DNA. The molecular docking technology predicts the best binding site and binding affinity between the complex and DNA, and then the catalytic mechanism of hydrolysis is supposed. The study results suggest that the Schiff base metal complex, as a potent artificial enzyme, may find its applications in catalytic hydrolysis and biotechnological areas.

***Keywords*:** Schiff base; complex; crystal structure; hydrolysis activity; catalytic mechanism

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