Experimental and molecular modeling studies of the interaction of the polypyridyl Fe(II) and Fe(III) complexes with DNA and BSA

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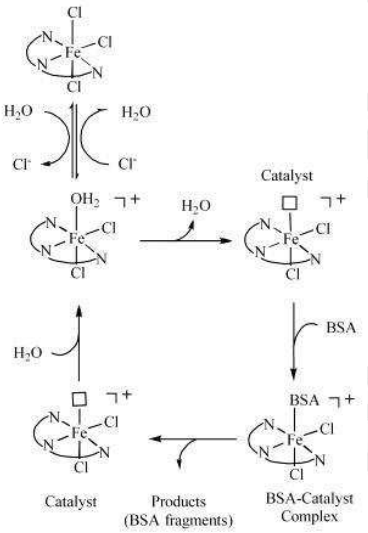
Two mononuclear iron complexes, $[Fe(tppz)_2](PF_6)_2 \cdot H_2O$ (1) and $Fe(tppz)Cl_3 \cdot 2CHCl_3$ (**2**) where tppz is (2,3,5,6-tetra(2-pyridyl)pyrazine), have been synthesized and characterized by elemental analysis, spectroscopic methods (UV–Vis and IR) and single crystal X-ray structure analysis. The interaction of (**1**) as the nitrate salt ($[Fe(tppz)_2](NO_3)_2$) with calf-thymus DNA (CT-DNA) has been monitored by UV–Vis spectroscopy, competitive fluorescence titration, circular dichroism (CD), voltammetric techniques, viscosity measurement, and gel electrophoresis. Gel electrophoresis of DNA with $[Fe(tppz)_2](NO_3)_2$ demonstrated that the complex also has the ability to cleave supercoiled plasmid DNA. The results have indicated that the complex binds to CT-DNA by three binding modes, *viz.*, electrostatic, groove and partial insertion of the pyridyl rings between the base stacks of double-stranded DNA [1-2]. Molecular docking of $[Fe(tppz)_2](NO_3)_2$ with the DNA sequence $d(ACCGACGTCGGT)_2$ suggests the complex fits into the major groove. The water-insoluble complex (**2**) can catalyze the cleavage of BSA at 40°C. There are no reports of the catalytic effect of polypyridyl metal complexes on the BSA cleavage. Molecular docking of (**2**) with BSA suggests that, when the chloro ligands in the axial positions are replaced by water molecules, the BSA can interact with the Fe(III) complex more easily.

Interaction:



Scheme 1. A proposed simple mechanism for the catalytic effect of (**2**) on the cleavage of BSA.

References

[1] H. Hadadzadeh, M. Salimi, M. Weil, M.T. Behnamfar, F. Darabi, *Polyhedron.* 53 (2013) 179.
[2] K. Abdi, H. Hadadzadeh, M. Salimi, J. Simpson, A. Dehno Khalaji, *Polyhedron* 44 (2012) 101.