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Exploiting the biological efficacy of benzimidazole based Schiff base complexes with L-Histidine as a co-ligand: Combined molecular docking, DNA interaction, antimicrobial and cytotoxic studies(Article)

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Abstract

Four new metal complexes were synthesized and screened for their cytotoxic activity after sufficient assertion from the preliminary DNA binding studies. The metal complexes could bind to CT-DNA through intercalation binding mode. This has also been confirmed by the molecular docking studies. The DNA cleavage efficiencies of these complexes with pBR322 DNA were investigated by gel electrophoresis. The complexes were found to promote the cleavage of pBR322 DNA from the supercoiled form I to the open circular form II in the presence of an oxidizing agent (H₂O₂). The in vitro chemosensitivity of the studied complexes exhibits significant cytotoxic effects, compared to those reported for cisplatin. These findings represent a prompting to search for the probable interaction of these complexes with other cellular elements of fundamental consequence in cell proliferation. The in vitro anticancer activities indicate that the Cu(II) complex is active against the selected human tumor cell lines, and the order of in vitro anticancer activities is consistent with the DNA-binding affinities. Towards noncancerous cell line, Cu(II) complex exhibits very low toxicity. On the other hand all the complexes have been found to exhibit cytotoxic effects against cancerous cell lines with potency more than that of the widely used drug cisplatin and hence they have the potential to act as promising anticancer agents. Captivatingly, they are non-toxic to normal cell lymphocytes revealing that they are selective in killing only the cancer cells. © 2018 Elsevier Inc.

Author keywords

[Cytotoxicity](#) [DNA binding studies](#) [Gel electrophoresis](#) [Molecular docking](#) [Schiff base metal complexes](#)

Indexed keywords

EMTREE drug terms:

[benzimidazole](#) [cisplatin](#) [cupric ion](#) [fluconazole](#) [histidine](#) [hydrogen peroxide](#)
[kanamycin A](#) [Schiff base](#) [antineoplastic agent](#) [benzimidazole](#) [benzimidazole derivative](#)
[DNA](#) [histidine](#) [ligand](#) [Schiff base](#)

EMTREE medical terms:

[antibacterial activity](#) [antifungal activity](#) [antimicrobial activity](#) [antineoplastic activity](#) [Article](#)
[cancer cell line](#) [chemosensitivity](#) [circular dichroism](#) [drug cytotoxicity](#) [drug DNA interaction](#)
[drug efficacy](#) [human](#) [human cell](#) [in vitro study](#) [minimum inhibitory concentration](#)
[molecular docking](#) [nonhuman](#) [priority journal](#) [cell proliferation](#) [chemical structure](#)
[chemistry](#) [DNA probe](#) [dose response](#) [drug effect](#) [drug screening](#)
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(2024) *Inorganica Chimica Acta*

An, H.-L. , Duan, Y. , Chen, T.-T.

Crystallographic, spectroscopic, and antimicrobial activities of nickel(II) and cadmium(II) complexes with N-heterocycle: TD/DFT calculations and Hirshfeld surface analysis

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DNA Probes Dose-Response Relationship, Drug Drug Screening Assays, Antitumor
Electrochemical Techniques Gram-Negative Bacteria Gram-Positive Bacteria Histidine
Humans Ligands Microbial Sensitivity Tests Molecular Docking Simulation
Molecular Structure Schiff Bases Structure-Activity Relationship

Chemicals and CAS Registry Numbers:

benzimidazole, 51-17-2; cisplatin, 15663-27-1, 26035-31-4, 96081-74-2; fluconazole, 86386-73-4; histidine, 645-35-2, 7006-35-1, 71-00-1; hydrogen peroxide, 7722-84-1; kanamycin A, 25389-94-0, 59-01-8; DNA, 9007-49-2;

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