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# *In vitro* DNA binding, pBR322 plasmid cleavage and molecular modeling study of chiral benzothiazole Schiff–base–valine Cu(II) and Zn(II) complexes to evaluate their enantiomeric biological disposition for molecular target DNA

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**A B S T R A C T**

Bicyclic heterocyclic compounds *viz*. benzothiazoles are key components of deoxyribonucleic acid (DNA) molecules and participate directly in the encoding of genetic information. Benzothiazoles, therefore, represent a potent and selective class of antitumor compounds. The design and synthesis of chiral antitumor chemotherapeutic agents of Cu(II) and Zn(II), L– and –D benzothiazole Schiff base –valine complexes **1**a & **b** and **2a** & **b**, respectively were carried out and thoroughly characterized by spectroscopic and analytical techniques. Interaction of **1a** and **b** and **2a** and **b** with CT DNA by employing UV–vis, florescence, circular dichroic methods and cleavage studies of **1a** with pBR322 plasmid, molecular docking were done in order to demonstrate their enantiomeric disposition towards the molecular drug target DNA. Interestingly, these studies unambiguously demonstrated the greater potency of L– enantiomer in comparison to D–enantiomer.

***Keywords:*** Chiral Cu(II)/Zn(II) benzothiazole–valine complexes, enantiomeric discrimination with DNA, binding studies, Molecular docking studies

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