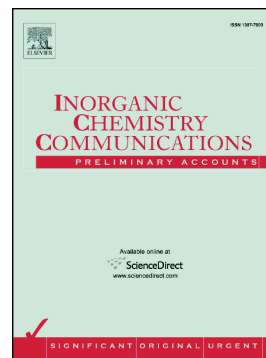


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# Synthesis, structural elucidation and dna binding profile of Zn(II) BIS-BENZIMIDAZOLE complexes

Mildred Rodriguez-Cordero,<sup>1</sup> Noelani Cigüela,<sup>1</sup> Ligia Llovera,<sup>2</sup> Teresa González,<sup>2</sup> Alexander Briceño,<sup>2</sup> Vanessa R. Landaeta,<sup>1</sup> Jesús Pastrán.\*<sup>1</sup>

<sup>1</sup>Departamento de Química, Universidad Simón Bolívar, Caracas, Venezuela.

<sup>2</sup>Centro de Química, Instituto Venezolano de Investigaciones Científicas, Miranda, Venezuela.

jpastran@usb.ve, Fax: +58 (0212) 906 3961

## ABSTRACT

Complexes of zinc (II) ( $\mathbf{L}^1\mathbf{ZnBr}_2$ ,  $\mathbf{L}^2\mathbf{ZnBr}_2$ ) were prepared in good yields using bis-benzimidazole ligands with olefinic bridges and different substituents on the nitrogen atoms in the benzimidazole cores ( $\mathbf{L}^1 = \text{H}$ ,  $\mathbf{L}^2 = \text{Bz}$ ). The crystal structure of  $\mathbf{L}^2$  was determined, showing that both benzimidazole rings and the carbon atoms of the olefinic bridge are coplanar with a slight deviation and that the benzyl substituent is perpendicular to this plane. Also, the crystal structure of  $\mathbf{L}^1\mathbf{ZnBr}_2$  was determined showing that in coordinated  $\mathbf{L}^1$ , benzimidazole rings are out the plane with respect to the olefinic bridge, allowing their coordination through the nitrogen atoms to get a strain-free seven-membered ring, achieving a distorted tetrahedral geometry. Both crystal structures of  $\mathbf{L}^2$  and  $\mathbf{L}^1\mathbf{ZnBr}_2$  exhibit  $\pi$ - $\pi$  stacking interactions that hold their supramolecular arrangement. All ligands and complexes were fully characterized. Additionally, through DNA binding studies using absorption spectral titrations it was possible to determine a slight hypochromism and bathochromism when ligands and complexes interact with calf thymus DNA in neat DMSO and 3% DMSO/Tris-HCl buffer, the spectral changes being consistent with partial intercalation. The intrinsic binding constant  $K_b$  of ligands and complexes are reported for each medium.

**Keywords:** bis-benzimidazole ligand; zinc complexes; CT DNA; binding constant.

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