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Synthesis and characterization of a zinc(II) complex bearing polyimidazole ligand with a medicinal approach

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β-lactam antibiotics play an essential role in intensive care, but their efficacy is often compromised by microbial resistance, especially through the action of β-lactamase enzymes, which inactivate these therapeutic agents. β-lactamases can be divided into two main groups: serine-β-lactamases, which include classes A, C and D, and metallo-β-lactamases (MBLs), which belong to class B[1]. Among these, MBLs are of particular interest, since effective inhibitors to reduce their enzymatic activity are still not available. Recently, polyimidazole ligands were employed in bioassays intending to hamper the zinc(II) network interactions in the active site of MBLs, where the addition of an electron-donating group to imidazole derivatives enhanced their inhibitory potency and facilitated the coordination of the zinc(II) ion[2]. Thus, the present work includes the synthesis and characterization of the complex [Zn(bmimahiscz)Cl] (*bmimahiscz* =((4,5-di((1-methyl-1H-imidazol-2-yl)methyl)-4,5,6,7-tetrahydro-1H-imidazo[4,5-c]pyridine)). The complex was synthesized by the reaction of *bmimahiscz* with $ZnCl_2$ in MeOH, at 25°C, and isolated as colorless single crystals by recrystallization in acetonitrile (yield= 49%). X-ray analysis revealed two distinct molecules in the unit cell, which are pentacoordinated assuming a geometry tending towards trigonal bipyramid (τ= 0.79/0.70). X-ray was pivotal to determine that the zinc (II) coordination promoted an open ring reaction in the ligand *bmimahiscz* resulting in the analogous tripodal *bmimahis* (2-(4H-3λ^4-imidazol-4-yl)-*N,N*-bis((1-methyl-1H-imidazol-2-yl)methyl)ethan-1-amine. Further analysis include IR (CsI): ν($CH_{arom/alif}$) 3140 - 2820; ν(C=N)/ (C=C) 1624 - 1457; ν(C-N_{amine}) 1287; δ (CH) 762 - 750; δ (Zn-$N_{imidazole}$) 254 in cm^{-1} and ESI-MS (DMSO, m/z^+): 408 (100%), 298 (67%, *bmimahiscz*), 442 (22%,[Zn(*bmimahiscz)*DMSO]$^{2+}$), 362 (4%, [Zn(*bmimahiscz*)]$^{2+}$). NMR techniques are being employed to understand the zinc(II) coordination to *bmimahiscz* and *bmimahis* ligands in solution and will be presented. At this point, the coordination of zinc(II) are only available with the *bmimahis* ligand bearing three imidazole groups that mimics the active site of the mononuclear MBL from Bacillus cereus (PDB1bmc).[3]

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