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BOOK OF ABSTRACTS

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A serendipitous product of the copper(II) famotidine reaction

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During the COVID pandemic many researchers found themselves looking to contribute to the search of active compounds against this coronavirus. One of the several strategies used was drug repositioning. In this context, antagonist H2 receptors, like famotidine, were targeted as potential active drugs. In our group, we worked on obtaining new coordination compounds of such antagonist H2 receptors. In this search, a solution of copper(II) chloride with a stoichiometric quantity of famotidine at a pH = 3 was left with constant stirring at 60 °C for 45 minutes. The resulting solution was left to slowly evaporate at room temperature until prismatic dark green crystals appeared. The obtained crystals were characterized by infrared spectroscopy, elemental analysis, thermogravimetric analysis and single crystal X-ray diffraction. The obtained structure showed that the famotidine had undergone a nucleophilic attack by a water molecule losing the terminal aminosulfonate group.

The compound crystallized at the monoclinic $P2_1/c$ space group with a = 6.94982(15), b = 12.3041(2), c = 17.4871(3) and β = 97.7421(18). The square pyramidal environment of the copper(II) center presents a equatorial N_2SCl coordination with two N and a S atom coming from the famotidine and a Cl completing the fourth position. Another Cl atom is coordinated in the apical position leading to a neutral compound.

Intermolecular interactions were analyzed using Hirshfeld Surfaces. Notably the structure is maintained by an extended H-bonding landscape including classical and non-classical H-bonds involving the water hydration molecule, the coordinated Cl, aminic N atoms and a carboxylic O from the terminal carboxylate group. The complexes form sheets through this H-bonding network along the *bc* plane.

Keywords: drug repositioning, famotidine, copper(II)

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