



Glucosamine and maltol anchored Zinc(II) complex of COVID-19 health supplement relevance: DFT collaborated spectroscopic formulation with profound biological implications

Jan Mohammad Mir^{a,b,*}, Bashir Ahmad Malik^a, Mohd Washid Khan^a

^a Department of PG Studies and Research in Chemistry and Pharmacy, RD University, Jabalpur, MP, India

^b Department of Chemistry, Islamic University of Science and Technology, Awantipora, India

ARTICLE INFO

Keywords:

Sugar
Zn(II)
Synthesis
DFT
SOD
Antimicrobial
Anti-covid

ABSTRACT

In association with other antiviral drugs, Zinc is specially administered to the patients suffering from novel coronavirus infectious disease (nCOVID). Zn, maltol, and glucosamine are famous food and drug additives. The supplements made from them are helpful in minimizing malnutrition problems, and in enhancing immune power. Due to the well-pronounced effects of all these three components in the food and medicinal industry, a novel sugar Zn(II) complex of the general composition, $[Zn(gls)(mal)]$, where Hmal is maltol and Hgls is referred to as glucosamine, was synthesized and formulated. The physicochemical methods that were used to establish the molecular structure include elemental analysis, ¹HNMR, FT-IR, UV-Vis., thermal and mass spectrometry. Physical properties like decomposition temperature and molar conductance were also examined. The experimental results at each step of characterization were validated/compared with density functionalized spectroscopic/spectrometric data using the LANL2DZ basis set for the metal atom and 6–31 g(d,p) for other atoms under the B3LYP functional. From the study, a suitable square planar geometry is suggested for the complex. Among biological implications, superoxide dismutation (SOD) and antimicrobial actions were studied. Also, virtual screening using SWISS ADME and Autodock 4.0 program (against 6X2B, SARS-CoV-2 u1S2q 2 RBD Up Spike Protein Trimer) were evaluated for the complex. Good interactions were scored by glucosamine and the complex. The results obtained from antimicrobial sensitivity indicate low inhibition zones, but from the SOD data, the complex has shown satisfactory antioxidant behavior. Therefore, the proposed food supplement could act as a good antioxidant agent and could keep the flora of the intestinal tract less disturbed while going through a metabolic pathway.

1. Introduction

Zinc is an “essential trace element” mainly used for the prevention of zinc deficiency [1], and is also known as intelligence mineral [2]. Zinc plays important role in the maintenance of normal human growth and health, and therefore zinc supplements are used to prevent or treat zinc deficiency [3,4]. Lack of zinc may result in poor vision and delayed wound healing [5,6]. Therefore, the evaluation of zinc as a shield against human health abnormalities like the common cold, ear/respiratory infections, malaria, macular degeneration, cataracts, asthma, diabetes, high blood pressure, acquired immune deficiency syndrome (AIDS), acne, etc has gained fascination [7,8]. Even the possible treatment of dreadful disorders like Alzheimer’s disease,

Crohn’s disease, Hansen’s disease, Down syndrome, and anorexia nervosa has been linked with this element [9,10]. Natural dietary Zn-sources include chicken, red meat, and cereals [11]. The recommended amount of daily intake of zinc lies in the range of 5.21–12.48 mg/day [12].

Glucosamine on the other hand possesses multifunctional therapeutic potential and is found naturally in the human body [13]. But with aging, a considerable decrease in the levels of this compound begins, slowly leading to the bone-joint breakage [14]. Like zinc, glucosamine is also available in the market in suitable supplement forms. Generally, glucosamine is found in two main types of salts *viz* hydrochloride and sulphate [15]. This compound helps to keep cartilage healthy [16]. Some experts believe that glucosamine sulphate may help counteract

* Corresponding author. Department of PG Studies and Research in Chemistry and Pharmacy, RD University, Jabalpur, MP, India.

E-mail address: mirjanmohammad@gmail.com (J.M. Mir).

<https://doi.org/10.1016/j.jics.2022.100743>

Received 1 July 2022; Received in revised form 14 September 2022; Accepted 18 September 2022

Available online 29 September 2022

0019-4522/© 2022 Indian Chemical Society. Published by Elsevier B.V. All rights reserved.