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Molecular Modeling of Chemicals Products Inhibitors of Growth Struvite Crystal

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Abstract

Struvite ($MgNH_4PO_46H_2O$) crystals were produced by infection associated with urea generating organisms.The aim of this study is to examine the interactions between the enzyme urease and two inhibitors, the first is an inhibitor monoatomic: Aluminum and the second is a polyatomic: Citrate by the methods of molecular modeling: molecular mechanics, molecular dynamics (MM^+, AMBER) and molecular docking (FleX). Supersaturated solutions induce crystallization by nucleation and subsequent crystal growth .The mechanisms for the formation of calcium phosphate urinary stones are still not understood. Chemicals product has been studied extensively as inhibitors and has been observed in the attachment of crystals to in vitro study. As a complement we have using an electron microscope Hitachi TM1000, we examined specimens of crystals struvite. The various figures show a set of grains of sizes of the order of 20 µm. The majority of these particles present regular forms. This suggests the crystal growing. This result to an alteration in the expression of these faces and the development of a characteristic architectural struvite morphology. Similar changes were observed in the presence of identical concentrations of citrate acid, and Alluminuium, emphasizing the unique interaction of phosphocitrate with the struvite crystal.

Keywords: Inhibitors, Struvite, Modeling, Interactions, Docking, MM, DM

1. Introduction

Infection lithiasis are composed primarily of magnesium ammonium phosphate hexahydrate ($MgNH_4PO_46H_2O$) but may, in addition, contain calcium phosphate in the form of carbonate apatite ($Ca_{10}[PO_4]6CO_3$) [1,2]. Infection of the urinary tract with urease-producing organisms is required for the formation of infection stones in humans. Although the species Enterobacteriaceae comprises the majority of urease-producing pathogens, a variety of gram-positive and gramnegative bacteria and some yeasts and mycoplasma species have the capacity to synthesize urease [3]. An elevated urinary pH reduces the solubility of magnesium ammonium phosphate and favors precipitation of Struvite crystals. Higher intake of phosphate (from Proteins) and magnesium based food and lower intake of water gives rise to the PO_4 3-and Mg^{2+} ions in the supersaturated urine, which leads to the conditions of formation of Struvite [4]. Probably, the negative charged points of the external side of the cellular structures could reduce the metastability field of struvite and calcite, acting as heterogeneous nuclei of crystallization [5]. For example, during digestion, are enzymes that accelerate the decomposition and food processing. An enzyme catalyzes only one reaction in general, because it is able to bind efficiently than a single substrate. This specificity results from the fact that when two molecules meet, their association may be stabilized by the establishment of a large number of weak bonds (hydrogen bonding, ionic bonding, Van Der Waals forces) these bonds are about 100 times weaker than a covalent bond. Modeling and simulation of struvite growth, incorporating solution chemistry and thermodynamics, growth kinetic and process description of the recovery system. An ensemble of experimental data is combined with the dynamic model to estimate struvite growth kinetics [6].

