

QM study of interaction between phthalocyanine silicone inhibitor and human α -carbonic anhydrase enzyme

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ABSTRACT

In the present study the electronic geometry of a novel silicon(IV) phthalocyanine bearing [(2E)-3-[4-(dimethylamino)phenyl]-1-(4-phenoxy)prop-2-en-1-one] group as a novel inhibitors of carbonic anhydrase enzyme was investigated theoretically. In continue the complexation between carbonic anhydrase enzyme center (CA) and silicon phthalocyanines inhibitor has been studied, based on, B3LYP level, using 6-31G* basis set. Predicted results indicate an exothermic interaction between this inhibitor and CA active center.

Keywords: Carbonic anhydrase, Silicon(IV) phthalocyanine, Inhibitor, QM study

1. INTRODUCTION

CA is a vital enzyme that catalyzes the rapid conversion of CO_2 to HCO_3^- and H^+ . CA isomers are found in a variety of tissues that are involved in several important biological processes such as basic acid balance, respiration, ion transport, and electrolyte excretion [1-3].

phthalocyanines, which are critical molecules for treating and detecting the use of various chemistry, biology, and pharmacology, especially water-soluble compounds, have the ability to bond with a very positive load, they can have wide range of antimicrobial and anticancer activity, Fig. 1 [4,5,9].

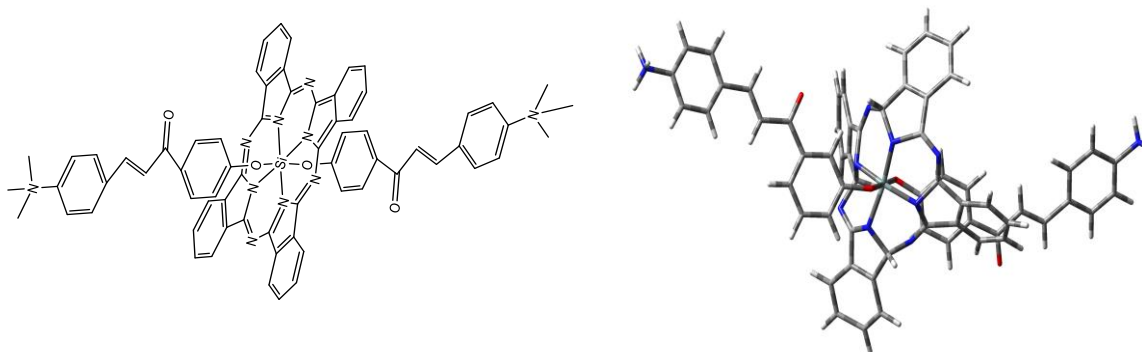


Fig.1. Chemical structure of the silicone phthalocyanines inhibitor (left) and optimized geometry of the silicone phthalocyanines inhibitor(right)