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LEAD OPTIMIZATION STUDIES ON NOVEL THIAZOLE DERIVATIVES AS CYP-450 INHIBITOR BY USING *IN-SILICO* MODULATION

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ABSTRACT

The *In-silico* studies considered as complementary to in vivo and in vitro biological studies are performed by using a computer and are playing increase larger and more important role in drug discovery and development. We describe here in *In-silico* study of various hypothetical Thiazole and their interactions with CYP450 enzymes by computational methods including chem draw ultra, Avogadro and ochem database software methods. We worked on a chemical reaction scheme of Thiazole and we prepared different 20 Thiazole derivatives. The CYP450 super family of heme enzymes plays an important role in the metabolism of a large number of endogenous and exogenous compounds including most of the drugs currently on the market. Comprehensive studies of the quantum approaches on the Thiazole derivatives like TD1, and TD18 was found to be CYP450 enzymes inhibitors interactions. The quantum approaches by lead optimization will require further studies; the data reported in this work may be helpful guide for medicinal chemist who is working in this area.

KEYWORDS: *In-silico*, Thiazole, CYP450 inhibitor

1. INTRODUCTION

Thiazole is an organic compound and the molecular formula C_3H_3NS. Thiazole is a heterocyclic compound featuring both a nitrogen atom and sulphur atom as part of the aromatic five-membered ring. Thiazole are related compound are called 1, 3-azoles (nitrogen and one other hetero atom in a five membered ring). Thiazoles obtained from microbial and marine origins exhibit antitumor and antiviral activities.[1,2] Thiazole being a key part of many