World Inventia Publishers

Journal of Synthetic and Natural Chemistry

http://www.worldinventiapublishers.com/JSNC/

Vol. 4, Issue 2, 2019

Research Article

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

Vishesh Kumar Maurya *and Himanshu Joshi

Invertis Institute of Pharmacy, Invertis University, Bareilly-243123, INDIA.

Received on: 10-03-2019; Revised and Accepted on 08-05-2019

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 Piperidine and their interactions with CYP450 enzymes by computational methods including chem draw ultra, Avogadro and achem database software methods. We worked on a chemical reaction scheme of Piperidine and we prepared different 20 Piperidine 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 Piperidine derivatives like P06 and P013 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, Piperidine, CYP450 inhibitor.*

INTRODUCTION

Piperidine is an organic compound with the molecular formula $(CH_2)_5NH$. This heterocyclic amine consists of a six-membered ring containing five methylene bridges (–CH_2–) and one amine bridge (–NH–). It is a colorless liquid with an odor described as objectionable, and typical of amines the name comes from the genus name piper which is the Latin word for pepper. Although piperidine is a common organic compound, it is best known as a representative structure element within many pharmaceuticals and alkaloids [1]. Piperidine is highly sterically hindered base, useful because of its low nucleophilicity and high solubility in organic solvents. Piperidine is found in barley. Piperidine is present in black pepper (Piper nigrum). Piperidine is a flavoring agent. Piperidine is an organic compound with the molecular formula $(CH_2)_5NH$. This heterocyclic amine consists of a six-membered ring containing five methylene units and one nitrogen atom. It is a colorless fuming liquid with an odor described as ammonical, pepper-like; the name comes from the genus name Piper, which is the Latin word for pepper. Piperidine is a widely used building block and chemical reagent in the synthesis of organic compounds, including pharmaceuticals. Piperidine is a widely used secondary amine. It is widely used to convert ketones to enamines. Enamines derived from piperidine can be used in the Stork enamine alkylation reaction. Piperidine is used as a solvent and as a base. The same is true for certain derivatives. N-formylpiperidine is a polar aprotic solvent with better hydrocarbon solubility than other amide solvents, and 2, 2, 6, 6 tetramethylpiperidine [2]. *In silico* literally Latin for "in silicon", alluding to the mass use of silicon for semiconductor computer chips is an expression used to mean performed on computer or via computer simulation. The phrase was coined in 1989 as an allusion to the Latin phrases in vivo, in vitro, and in situ, which are commonly used in biology and refer to experiments done in living organisms, outside of living organisms, and where they are found in nature, respectively [3]. Computer-aided drug design is the use of computer systems to aid in the creation, modification, analysis, or optimization of a design. CADD software is used to increase the productivity of the designer, improve the quality of design, improve communications through documentation, and to create a database for manufacturing [4]. CADD output is often in the form of electronic files for print, machining, or other manufacturing operations. Its use in designing electronic systems is known as electronic design automation. In mechanical design it is known as mechanical design automation or computer-aided drafting, which includes the process of creating a technical drawing with the use of computer software [5]. Inhibitors of the CYP450 enzymes have more important role in the treatment of several disease conditions such as numerous cancers and anti fungal interactions in addition to their critical role in drug-drug interaction. Understanding the key structure features of

***Corresponding author:**

Vishesh Kumar Maurya

Invertis Institute of Pharmacy,

Invertis University, Bareilly-243123, INDIA.

**E-Mail: Visheshmaurya97@gmail.com*

DOI: https://doi.org/10.5281/zenodo.2793315