More et al., 1:9
http://dx.doi.org/10.4172/scientificreports.439

Open Access Scientific Reports

Research Article Open Access

%PDLJOH 4UVEJFT PG #FO[JNJEB[PMF %FSJWB "$$BTF *OIJCJUPS

Poonam M More[1]*, Rishikesh V Antre[1], Tushar T Shelke[1], Madhavi M Mutha[1], Sahar M Badr[2], Hassan M Eisa[2] and Pradeep V Kore[1]

[1]*Medicinal Chemistry Research Laboratory, JSPM'S Charak College of Pharmacy and Research, Pune, Maharashtra, India*
[2]*Department of Organic Chemistry, Faculty of Pharmacy, Mansoura, Egypt*

Abstract

In these continuing efforts towards the development of disease modifying treatment for microbial diseases, we are targeting acetyl coenzyme-A carboxylase (ACCase) and it is essential for pathogen survival. In present study we reported the docking studies of substituted benzimidazole derivatives with acetyl coenzyme-A carboxylase inhibitor.

Keywords: Acetyl coenzyme-A carboxylase inhibitor (Accase); Benzimidazole; Antimicrobial activity

Introduction

Benzimidazole [1] is a heterocyclic aromatic organic compound. This bicyclic compound consists of the fusion of benzene and imidazole. Benzimidazole derivatives play important role in medicinal field. Benzimidazole derivatives have found the application in diverse therapeutic areas including antimicrobial activity [2,3], the activity against several viruses such as HIV [4,5], antiallergic [6,7], antioxidant [8], antihistaminic [9], antibacterial [10], anti-diabetic [11], antifungal [12] activity.

Many researchers have concentrated on the development of inhibitors of ACCase inhibitors as antimicrobial activity. Several bacteria such as gram positive, gram negative bacteria are responsible

***Corresponding author:** Poonam M More, Medicinal Chemistry Research Laboratory, JSPM'S Charak College of Pharmacy and Research, Pune, 412 207, Maharashtra, India, E-mail: rishiantre@gmail.com

Received September 26, 2012; **Published** October 27, 2012

Citation: More PM, Antre RV, Shelke TT, Mutha MM, Badr SM, et al. (2012) Docking Studies of Benzimidazole Derivatives as Coenzyme-A Carboxylase (ACCase) Inhibitor. 1:439. doi: V F L H Q W L ¿ 9 F U H S R U W V

Citation: More PM, Antre RV, Shelke TT, Mutha MM, Badr SM, et al. (2012) Docking Studies of Benzimidazole Derivatives as Coenzyme-A Carboxylase (ACCase) Inhibitor. 1:439. doi: V F L H Q W L ¿ F U H S R U W V

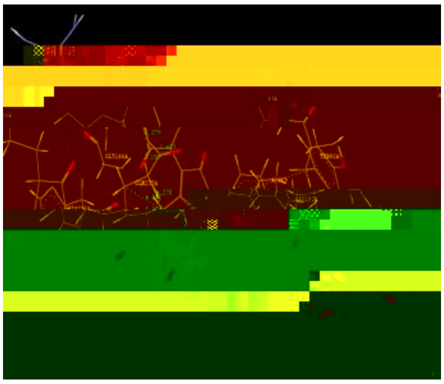

Figure 2f: Hydrogen bonding and hydrophilic interaction of 15A ligand molecule.

Figure 2g: Hydrogen bonding and hydrophilic interaction of 21A ligand molecule.

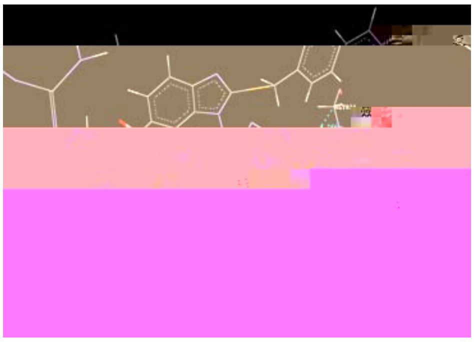

Figure 2h: Hydrogen bonding and hydrophilic interaction of 23A ligand molecule.

receptor is removed further. From this predicted docked this complex and selected ligand and receptor to check their interaction.

Result and Discussion

Focused compound screening libraries are being used to improve the efficiency and productivity of early drug discovery. Traditionally each compound in a focused library is selected based on potential physical properties that will increase its probability of having activity for a specific target. In this study we have extended this approach in order to identify potential non-ligands as inhibitors. Following are the active residues involved in docking (Figures 1-3) (Table 1).

Citation: More PM, Antre RV, Shelke TT, Mutha MM, Badr SM, et al. (2012) Docking Studies of Benzimidazole Derivatives as Coenzyme-A Carboxylase (ACCase) Inhibitor. 1:439. doi: VFLHQWL¿FUHSRUWV

Figure 3e: Ligand molecule 7a docked in cavity no.1 of PDB (3JZI).

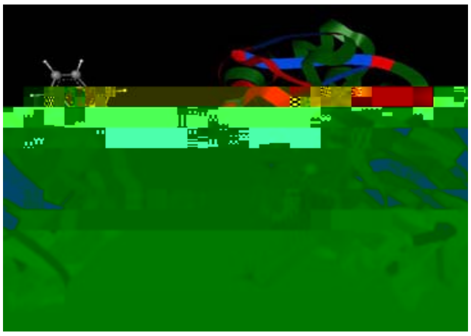

Figure 3f: Ligand molecule 9D docked in cavity no.1 of PDB (3JZI).

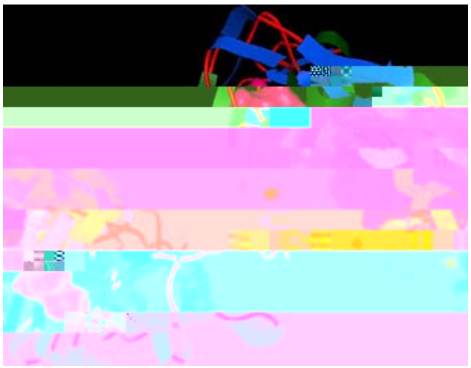

Figure 3g: Ligand molecule 21A docked in cavity no.1 with assorted representation of PDB (3JZI). 7KH ¿JXUHV D K VKRZV WKH +\GURJHQ bond interaction in green color and the hydrophobic interaction blue color. 7KH ¿JXUHV D J VKRZV WKH OLJDQG PROHFXOH GRFNHG LQ FDYLW\ QR ZLWK WKH receptor. The logP value (Table 1) of ligands 9E, 12A, 15A shows the very less as compared with other ligands, because 9E, 12A and 15A contains two carbonyl group substitution. Although, the substituted elucidated, molecular docking experiments indicates that ligand binds at active site residue only SUHGLFWHG E\ %LRSUHGLFWD !!9/LIH0'6 DV VKRZQ LQ ¿JXUH D

Conclusion

To conclude, this is the report relating the antimicrobial activity with acetyl coenzyme A carboxylase inhibition and describing the binding site of protein. For protein ligand interaction as the base deduces it reveals that ARG292A, TYR82A, GLY83A, GLY165A, GLY166A, HIS236A, GLN 237A, LYS238A, VAL295A are involved in molecular docking. In conclusion, we have developed a novel series of benzimidazole as 9B, 9D,

anti-asthmatic activitives of some novel benzimidazole derivatives. J Chem Pharma Res 2: 215-224.

2. Ozden S, Atabey D, Yildiz S, Göker H (2005) Synthesis and potent antimicrobial activity of some novel methyl or ethyl 1H-benzimidazole-5-carboxylates derivatives carrying amide or amidine groups. Bioorg Med Chem 13: 1587-1597.

3. Sztanke K, Pasternak K, Sidor-Wojtowicz A, Truchlinska J, Jozwiak K (2006) Synthesis of imidazoline and imidazo[2,1-c][1,2,4]triazole aryl derivatives containing the methylthio group as possible antibacterial agents. Bioorg Med Chem 14: 3635-3642.

4. Porcari AR, Devivar RV, Kucera LS, Drach JC, Townsend LB (1998) Design, synthesis, and antiviral evaluations of 1-(substituted benzyl)-2-substituted-5,6-