

NEW 2,4,5-TRISUBSTITUTED-1,3-THIAZOLE DERIVATIVES: SYNTHESIS, IN VITRO ANTIMICROBIAL ACTIVITY AND IN SILICO STUDY

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Abstract

A series of thiazole derivatives 1-4 were synthesized employing simple one-pot reaction pathway and characterized via Fourier Transform Infrared (FTIR), Proton Nuclear Magnetic Resonance (H-1 NMR), Ultraviolet-Visible (UV-Vis) and Gas Chromatography-Mass Spectrometry (GC-MS). The newly synthesized compounds were evaluated for their in vitro antimicrobial properties against several bacterial strains including Gram-positive and Gram-negative as well as fungus using broth microdilution method. The results revealed that all of the compounds exhibited good activity with a range of MIC values between 1.25-5.0 mg/mL. From the MIC and MBC results, compound 1 exhibited good activities with same MIC value of 1.25 mg/mL and MBC value of 5 mg/mL against B. cereus and S. flexneri. In order to support antimicrobial results, the molecular docking studies were carried out for inhibition of the GlcN-6-P synthase as the target. Out of four compounds underwent for molecular docking studies, 5-acetyl-4-methyl-2-(4-aminobiphenyl)-1,3-thiazole (1) shows the lowest minimum binding energy at -7.32 kcal/mol as compared to 2, 3 and 4 with -7.31, -7.20 and -6.76 kcal/mol, respectively which are in agreement with antimicrobial assay results. In conclusion, 2, 4, 5-trisubstituted-1,3-thiazole derivatives could be considered as promising antimicrobial in drug discovery candidates.

Keywords

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1. [Synthesis and Evaluation of Selected Benzimidazole Derivatives as Potential Antimicrobial Agents](#) Times Cited: **35**
 By: Alasmary, Fatmah A. S.; Snelling, Anna M.; Zain, Mohammed E.; et al.
 MOLECULES Volume: 20 Issue: 8 Pages: 15206-15223 Published: AUG 2015

2. [Syntheses, spectral characterization, single crystal X-ray diffraction and DFT computational studies of novel thiazole derivatives](#) Times Cited: **18**
 By: Anbazhagan, R.; Sankaran, K. R.
 JOURNAL OF MOLECULAR STRUCTURE Volume: 1050 Pages: 73-80 Published: OCT 24 2013

3. [Facile one-pot multicomponent synthesis and molecular docking studies of steroidal oxazole/thiazole derivatives with effective antimicrobial, antibiofilm and hemolytic properties](#) Times Cited: **10**
 By: Ansari, Anam; Ali, Abad; Asif, Mohd; et al.
 STEROIDS Volume: 134 Pages: 22-36 Published: JUN 2018

4. [EVALUATION OF THE ANTIMICROBIAL AND ANTI-BIOFILM ACTIVITY OF SOME 4,2 AND 5,2 BISTHIAZOLES DERIVATIVES](#) Times Cited: **14**
 By: Aranciu, C.; Marutescu, L.; Oniga, S.; et al.
 DIGEST JOURNAL OF NANOMATERIALS AND BIOSTRUCTURES Volume: 9 Issue: 1 Pages: 123-131 Published: JAN-MAR 2014

5. [Synthesis, molecular docking and QSAR studies of 2, 4-disubstituted thiazoles as antimicrobial agents](#) Times Cited: **10**
 By: Arora, P.; Narang, R.; Bhatia, S.; et al.
 J Appl. Pharm. Sci. Volume: 5 Issue: 2 Pages: 28-42 Published: 2015
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6. [Recent applications of 1,3-thiazole core structure in the identification of new lead compounds and drug discovery](#) Times Cited: **130**
 By: Ayati, Adile; Emami, Saeed; Asadipour, Ali; et al.
 EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY Volume: 97 Pages: 699-718 Published: JUN 5 2015

7. [Methods for in vitro evaluating antimicrobial activity: A review](#) Times Cited: **936**
 By: Balouiri, Mounyr; Sadiki, Moulay; Koraichi Ibensouda, Saad
 JOURNAL OF PHARMACEUTICAL ANALYSIS Volume: 6 Issue: 2 Pages: 71-79 Article Number: 2095-1779(2016)6:2<71:MFIVEA>2.0.TX;2-H
 Published: APR 2016

8. [One-pot Synthesis and Characterization of Highly Functionalized Thiazoles](#) Times Cited: **4**
 By: Beyzaei, Hamid; Beygi, Adel; Aryan, Reza
 IRANIAN JOURNAL OF CHEMISTRY & CHEMICAL ENGINEERING-INTERNATIONAL ENGLISH EDITION Volume: 35 Issue: 4 Pages: 31-37
 Published: FAL 2016

9. [Synthesis and Anticancer Activity of Novel Thiazole-5-Carboxamide Derivatives](#) Times Cited: **9**
 By: Cai, Wen-Xi; Liu, Ai-Lin; Li, Zheng-Ming; et al.
 APPLIED SCIENCES-BASEL Volume: 6 Issue: 1 Article Number: UNSP 8 Published: JAN 2016

10. [2-Aminobenzothiazole derivatives: Search for new antifungal agents](#) Times Cited: **43**
 By: Catalano, Alessia; Carocci, Alessia; Defrenza, Ivana; et al.
 EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY Volume: 64 Pages: 357-364 Published: JUN 2013

11. [Synthesis and antiviral activity of some new bis-1,3-thiazole derivatives](#) Times Cited: **31**
 By: Dawood, Kamal M.; Eldebss, Taha M. A.; El-Zahabi, Heba S. A.; et al.
 EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY Volume: 102 Pages: 266-276 Published: SEP 18 2015

12. [Synthesis and study of 1,3,5-triazine based thiazole derivatives as antimicrobial agents](#) Times Cited: **21**
 By: Desai, N. C.; Makwana, Atul H.; Rajpara, K. M.
 JOURNAL OF SAUDI CHEMICAL SOCIETY Volume: 20 Supplement: 1 Pages: S334-S341 Published: SEP 2016