18th National and 3rd International Conference of Iranian Biophysical chemistry

هجدهمین همایش ملی و سومین همایش بین المللی بیوشیمی فیزیک ایران

25-26 Des, 2024, University of Hormozgan

۶-۵ دی ماه ۱۴۰۳، دانشگاه هرمزگان

Synthesis of new β-lactams contain anthraquinone and their molecular docking

Maaroof Zarei *, Raheleh Jamalinasab, Masoud Mohamadzadeh

Department of Chemistry, Faculty of Sciences, University of Hormozgan, Bandar Abbas ۷۱۹۶۱, Iran. E-mail: mzarei@hormozgan.ac.ir, mzarei۵۷@gmail.com

Abstract

β-Lactam antibiotics are the most important antibacterial agents for human health and it began with the discovery of penicillin by Alexander Fleming in ۱۹۲۸. In addition, β-lactams are an important class of heterocyclic compounds due to their wide range of applications in other biological activities. With the alarming trends in bacterial resistance to many β-lactam antibiotics it has become necessary to synthesize novel β-lactams for bioassay of antibacterial activity and the need for drugs with more specific antibacterial activity. Therefore, the synthesis of the new β-lactams is the subject of extensive study. The anthraquinone and related compounds have been represented as a broad and growing family of bioactive molecules. Novel β-lactams contain anthraquinone on C-۳ position were synthesized by ketene-imine cycloaddition and characterized by spectral data. Molecular docking studies were carried out by Autodoc software. Penicillin-binding protein ۲a (PDB ID: ۱VQQ) from methicillin-resistant Staphylococcus aureus strain used as a target which good binding interactions were observed. In silico molecular docking studies of novel β-lactam-anthraquinone hybrids showed moderate to excellent interactions. Some of the synthesized β-lactams have lower binding energy than penicillin G. The overall interaction may be attributed to the presence of β-lactam ring and anthraquinone moiety.

Key words: β-lactam, anthraquinone, antibacterial, bacterial resistance, molecular docking

References

[۱] Güleç, Ö., Türkeş, C., Arslan, M., Demir, Y., Dincer, B., Ece, A., Beydemir, Ş. Novel beta-lactam substituted benzenesulfonamides: in vitro enzyme inhibition, cytotoxic activity and in silico interactions. Journal of Biomolecular Structure and Dynamics, ٤٢(١٢): ٦٣٥٩-٦٣٧٧, ٢٠٢٤.

[۲] Zarei, M., Mohamadzadeh, M. ۳-Thiolated ۲-azetidinones: synthesis and in vitro antibacterial and antifungal activities, Tetrahedron, ٦٧(٣٢), ٥٨٣٢-٥٨٤٠, ٢٠١١.

[۳] Zarei, M., Utilization of DMF-PhCOCl adduct as an acid activator in a new and convenient method for preparation of β-lactams, Bulletin of Chemical Society of Japan, ۸۵(۳), ۳٦۰-۳٦۸, ۲۰۱۲.

[٤] Aris , P., Mohamadzadeh, M., Zarei, M., Xia, X. Computational design of novel Griseofulvin derivatives demonstrating potential antibacterial activity: Insights from molecular docking and molecular dynamics simulation, International Journal of Molecular Sciences, ۲۵(۲), ۱۰۳۹, ۲۰۲٤.