Phosphorus, Sulfur, and Silicon and the Related Elements ›
Volume 196, 2021 - Issue 3

Articles

Synthesis and molecular design of mono aspirinate thiourea-azo hybrid molecules as potential antibacterial agents

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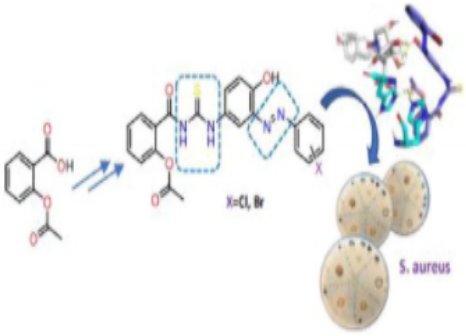
Pages 275-282 | Received 15 Jun 2020, Accepted 23 Sep 2020, Published online: 08 Oct 2020

Download citation | https://doi.org/10.1080/10426507.2020.1828885

Abstract

New mono aspirinate thiourea-azo derivatives **2a–f** were synthesized using aspirin as a natural product-based precursor, with 4-aminophenylazophenol derivatives in excellent 70–90% yields. Overall, **2a–f** gave excellent antibacterial activity against *Staphylococcus aureus* S48/81 and 2-(((3-((2-bromophenyl)diazenyl)-4-hydroxyphenyl)carbamothioyl)carbamoyl)phenyl acetate **(2d)** exhibited a larger zone of inhibition 10 mm, comparable to the standard ampicillin. The molecular docking analysis of **2d** against *S. aureus* tyrosyl-tRNA synthetase protein displayed a free energy interaction of −7.7 kcal/mol compared to aspirin (−6.4 kcal/mol).



Keywords: Aspirin | molecular docking | *S. aureus* | *E. coli* | antimicrobial

‹ Previous article | View issue table of contents | Next article ›