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Organotin (IV) Based Complexes as Promiscuous Antibacterials: Synthesis in vitro, in Silico Pharmacokinetic, and Docking Studies

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Abstract : Five novel triorganotin (IV) compounds have been synthesized and characterized. The tin atom is penta-coordinated to assume trigonal-bipyramidal geometry. Using in silico derived parameters; the objective of our study is to design and synthesize promiscuous antibacterials potent enough to combat resistance. Among various synthesized organotin (IV) complexes, compound 5 was found as potent antibacterial agent against various bacterial strains. Further lead optimization of drug-like properties was evaluated through in silico predictions. Data mining and computational analysis were utilized to derive compound promiscuity phenomenon to avoid drug attrition rate in designing antibacterials. Xanthine oxidase and human glucose- 6-phosphatase were found as only true positive off-target hits by ChEMBL database and others utilizing similarity ensemble approach. Propensity towards a-3 receptor, human macrophage migration factor and thiazolidinedione were found as false positive off targets with E-value 1/4> 10^-4 for compound 1, 3, and 4. Further, displaying positive drug-drug interaction of compound 1 as uricosuric was validated by all databases and docked protein targets with sequence similarity and compositional matrix alignment via BLAST software. Promiscuity of the compound 5 was further confirmed by in silico binding to different antibacterial targets.

Keywords : antibacterial activity, drug promiscuity, ADMET prediction, metallo-pharmaceutical, antimicrobial resistance
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