Diindolylmethane (DIM) Bearing Thiadiazole And Benzofuran-Based-Thiazoldinone Analogues as Urease Inhibitors: Design, Synthesis, Their In Vitro Potential and In Silico Studies

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Abstract

Urease (EC 3.5.1.5) belongs to the family of amidohydrolase enzymes having two nickel atoms in their core structure. Urease involves the conversion of urea into ammonia and carbon dioxide or carbamate. Urease is broadly found in nature and bio-synthesized by different organisms such as plants, fungi, bacteria, invertebrates, algae and are found in soil as soil enzyme. The current study describes synthesis of diindolylmethane (DIM) derivatives based-thiadiazole and benzofuran-based-thiazoldinone analogues as a new class of urease inhibitors. Diindolylmethane is natural product alkaloid reported to use in medicinal chemistry extensively. Diindolylmethane-based-thiadiazole and benzofuran-based-thiazoldinone analogues were synthesized and characterized by various spectroscopic techniques 1HNMR, 13C-NMR, HREI-MS and evaluated for urease (jack bean urease) inhibitory potential. All compounds showed excellent to moderate inhibitory potential having IC50 values within the range of 0.50 ± 0.01 to 33.20 ± 1.20 µM compared with the standard thiourea (21.60 ± 0.70 µM). A structure-activity relationship (SAR) of this series has been established based on electronic effects and position of different substituents present on phenyl rings. The key binding interactions of most active compounds with enzyme were confirmed through molecular docking studies. It was inferred that some of these potent urease inhibitors might serve as novel templates in drug designing.

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OH-MySanitiser

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Abstract

Washing your hands is the best way to prevent the spread of germs, but you don't always have access to soap and water. Hand sanitizer and hand cleansers have become a hot commodity since the pandemic began. After an initial drought—companies are rolling out new options to keep up with the demand. It's always good to have extra hand sanitizer around for when the need arises. Our product, OH-MySanitiser is a great alternative for quick, on-the-go cleaning. For on-the-go, nothing beats single-use hand sanitizers you can fit in your purse or even your pocket. OH-MySanitiser is a single-use item stored in a breakable liquid capsules that could be easily dispensed as needed, saving the need to carry around full bottles of sanitizer, allows user to discreetly and frequently sanitise hands from common bacteria, viruses or biological agents, durably carried in a pocket. The capsule encapsulating the rinse free waterless sanitising gel is made up of polymer that solubilises upon contact with hands. Popping the capsule inside clenched hands releases a measured, optimum amount of hand sanitiser. OH-MySanitiser would dispose the need for large bulky storage, and prevent spillage. The encapsulated single use packaging prevents unwanted evaporation of alcohol and thus keeping an ideal composition for optimal sanitising purpose. Additionally, disposable and degradable gel capsule reduces plastic waste and pollution.

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