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INSIGHTS ON Sip-B ACTIVE SITE AND ITS INHIBITORS: AN IN SILICO APPROACH

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Abstract

Salmonella enterica serovar Typhi (S. Typhi) and S. Paratyphi, namely typhoidal Salmonellae, are the cause of (para) typhoid fever, which is a devastating systemic infectious disease in humans. Salmonella enterica possesses two virulence-related type III secretion systems that deliver more than forty effectors. Type III secretion systems are molecular machines used by many Gram-negative bacterial pathogens to inject proteins, known as effectors, directly into eukaryotic host cells. SipB, SipC, and SipD are a group of proteins known as translocators that are themselves secreted through T3SS1. The cell invasion protein, SipB has been identified as a potential target which is known to be involved in important functions like host cell entry, transfer of other effector proteins into the host cell, inducing macrophage apoptosis, activating proapoptotic enzyme Caspase I for inducing autophagy. Inhibitors of SipB can be developed as potential anti virulent agents. Currently, 75 natural compounds have been identified as inhibitors of SipB. In this review we compiled inhibitors of Sip-B and identified their important interactions and structural characteristics required on the active site of Sip B using Autodock.

Key words: In silico, SipB, autodock, antivirulent.

PHYTOCHEMICAL SCREENING AND ANTI-INFLAMMATORY ACTIVITY OF CENTELLAASIATICA

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Abstract

Centellaasiatica is a valuable medicinal herbaceous aromatic creeper which has been valued for centuries in ayurvedic medicine. Phytochemical analysis of *Centellaasiatica* (Apiaceae) plant extracts revealed the presence of various biochemical compounds such as alkaloids, flavonoids, glycosides, phenolic compounds, triterpenoids and saponin etc. Since phenolic compounds, triterpenoids and flavonoids have remarkable anti-inflammatory, anti-arthritic and antioxidant activities, so our present work aims at evaluating the in vitro anti-inflammatory activity by Human Red Blood Cell (HRBC) membrane stabilization. The inhibition of hypotonicity induced HRBC membrane lysis was taken as a measure of the anti-inflammatory activity. The maximum membrane stabilization of *Centellaasiatica* extracts was found to be 94.97% at a dose of 2000 µg/ml. The results show that the extracts of *Centellaasiatica* exhibited anti-inflammatory activities. *Centellaasiatica* is a profusely branched prostate herb consisting of active principles such as Vallarine, Asiaticoside, Sitosterol, Tannins, Oxy - asiaticoside. Asiaticoside is used in the treatment of leprosy. Sitosterol and tannin possess antiprotozoal and spasmolytic property. According to Siddha literature, its leaves are used in the treatment of syphilis, all types of fever, children's abdominal disorder, elephantiasis and hydrocele and these features are highlighted in this article.

Keywords: Centellaasiatica, Anti-inflammatory, HRBC membrane stabilization.

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