عنوان مقاله:

Anti-Helicobacter pylori Potential of Podophyllotoxin : In Silico Study

محل انتشار:

مجله بین المللی میکروبیولوژی مولکولی و بالینی, دوره 12, شماره 1 (سال: 1401)

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خلاصه مقاله:

Helicobacter pylori is probably the most common chronic bacterial infection in humans and has infected almost half of the world's population. Podophyllotoxin is a lignan compound of plant origin and has great medicinal importance due to its various biological properties. The aim of this study was to investigate the podophyllotoxin as Urease, VacA and cagA inhibitor of Helicobacter pylori. The crystallized structure of podophyllotoxin was received from the Zinc database and used as a ligand. The structure of the ligand was optimized by the mm۲ method with Chem۳D v۲۰.۱.۱.۱۲۵ software. The ligand was evaluated as an inhibitor against the active site of the urease enzyme, VacA, and cagA by AutodackVina software. The output results were analyzed and evaluated by Discovery Studio v۱۶.۱.۰ software. The best affinity was obtained against VacA = -۸.۱ kcal/mol. The highest diversity of links was also reported in VacA. Hydrogen bonds established with VacA against tyrosine=۷۲۹ and threonine=۶۷۲, indicating the effectiveness of podophyllotoxin against VacA. Podophyllotoxin against cagA and Urease also showed a variety of hydrogen bonds respectively with lysine, serine, and tyrosine - glutamine, arginine, and asparagine. These results demonstrate the excellent inhibition of podophyllotoxin against Helicobacter pylori. Helicobacter pylori plays a key role in the development of gastric cancer. The transplant conformations predicted in this study showed that podophyllotoxin has valuable inhibitory potential. Therefore, podophyllotoxin may be considered as an anti- Helicobacter pylori agent for further research into drug development.

کلمات کلیدی:

Helicobacter pylori, Podophyllotoxin, Urease, VacA protein, cagA protein