

عنوان مقاله:

In silico modeling and characterization of Lasparaginase from bacteria, plants and fungal sources, using computational tools and online servers

محل انتشار:

بیستمین کنگره ملی و هشتمین کنگره بینالمللی زیستشناسی ایران (سال: 1397)

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خلاصه مقاله:

L-Asparaginase as a chemotherapeutic agent plays a very important role in the treatment of patients with acute lymphocytic leukemia)ALL), chronic myeloid leukemia (CML) and Hodgkin s lymphoma. In this study, in order to find resistant structures or less susceptibility to cysteine, the first, second and third structure of the protein, molecular weight and isoelectric point of the enzyme were investigated in three sources of bacterial, herbal and fungal .Asparaginase enzyme from the origin of bacteria Escherichia coli and Campylobacter jejuni, an herb of Withania somnifera and fungus, Fusarium equiseti was studied. Amino acid sequences were extracted from the NCBI site. The second structure was studied using the software Psipred and the third structure through SWISS-MODEL software. To evaluate the domain function, PROSITE software was used. The molecular weight, isoelectric point and the number and types of amino acids of the asparaginase structure in the studied origins were obtained from isoelectric.ovh.org site. The results showed a significant difference in nucleotide, amino acid, and the number of alpha and beta structures and the third structures of protein in the studied sources. But significantly, the asparaginase enzyme in the three studied sources had functional indices such as the domain performance, molecular weight, and the same isoelectric domain, which could confirm the Codon usage phenomenon. Regarding the sensitivity of this enzyme to the cysteine-proteases, it is important to find the structures of asparaginase without cysteine or low cysteine amino acids in comparison with asparaginases with prokaryotic and eukaryotic origin. Asparaginase enzyme in E.coli has 2 cysteines, C.jejuni without cysteine, 4 cysteines in Withania somnifera and 6 cysteines in Fusarium equiseti. In this study, by comparing the structures of asparaginase, an appropriate structure for in vitro studies, such as genome editing, has been attempted to produce a higheryielding drug. Investigating the structural and functional characteristics of this enzyme can be useful in optimizing the design of the drug and eliminating its side effects, in .addition to providing more information about functional and structural characteristics

كلمات كليدى:

L-Asparaginase, Acute lymphoblastic leukemia, In silico

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