

پزشکی شخصی

زنان و بهداشت باروری

ژنتیک پزشکی

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نانو زیست فناوری پزشکی

میکروپ شناسی و بیماری های عفونی

مهندسی بافت و سلول های بنیادی

سرطان؛ پیشگیری، تشخیص و درمان

متابولیسم و بیماری های متابولیکی

2nd International Congress on Biomedicine

ICB 2018

دومین کنگره بین المللی زیست پزشکی

پرمخاطب ترین کنگره بین المللی پزشکی در ایران

۳ لغایت ۶ دی ماه ۱۳۹۷ - سالن همایش میلاد، نمایشگاه بین المللی تهران

با امکان شرکت در کنگره به صورت حضوری و غیر حضوری



دانشگاه علوم پزشکی
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دریافت گواهینامه با اعتبار بین المللی از مرکز استاندارد علمی سوئیس
با تایید دانشگاه علوم پزشکی تهران، دانشگاه آزاد، پژوهشگاه رویان و انستیتو نسیم
از طرف دبیرخانه دومین کنگره بین المللی زیست پزشکی

با حداکثر ۲۰ امتیاز بازآموزی | گواهینامه عالی بین المللی

۰۲۱۳۶۲۰۸۹۰۹-۲۶۳۰۹۷۴۱

ثبت نام
www.icb2018.com



In silico comparison of binding of lactoferrin from different species to receptors involved in the development of cognitive function in infants

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Abstract

Introduction

Mothers milk is recommended for all newborn children. nonetheless, in some cases, breastfeeding is insufficient or unsuccessful or harmful for some medical reasons, or the mother decides not to bosom feed either at all or for a time. infant feeding formulas have been developed for these circumstances. immediate feeding formulas are widely used today to provide supplemental or sole source nutrition. recently, studies shown that breastfeeding may provide cognitive advantages. however, the connection between breast feeding and cognitive development is unclear. it was shown that lactoferrin (Lf) might have a significant role as a contingent nutrient for the brain development and development of cognitive function in infants. thus, it was hypothesized that Lf crosses the blood-brain barrier through a high affinity brain lactoferrin receptor (lrp) pathway. other studies suggested that lactoferrin might bind to a specific receptor on the brush border membrane, intelectin, to modulate autonomic nervous activity. lactoferrin is a glycoprotein with a molecular weight of about 80 kda, which binds to two iron atoms with high affinity. Lf is found in mucosal secretions, including tears, saliva, vaginal fluid, semen, nasal and bronchial secretions, bile, gastrointestinal fluids, urine and most highly in milk and colostrum. this glycoprotein is one of the innate immune system components with broad range of antimicrobial activates comprising antiviral, antibacterial, antifungal and also anti-cancer and immunomodulatory actions. the objective of this study was to compare binding of different Lf to brain lactoferrin receptors and intelectin by protein-ligand docking.

Methods

The crystal structures of human, horse, cattle, goat, buffalo and single-humped camel lactoferrin were retrieved from the uniprot (www.uniprot.org). the protein structure of sheep, zebo cattle and double-humped camel Lf were predicted by the i-tasser server, and then the results were validated



using saves v5.0 server. the crystal structures of lrp and intelectin receptors obtained from protein data bank (www.rcsb.org) then the pdb files prepared for docking calculation. cluspro server was used for protein docking. all of parameters were considered as their default values, and in all docking studies, ligand was allowed to be flexible.

Results

In this study, we showed that the lf can bind to specific receptors involved in the development of cognitive function, thus lactoferrin might have an effect on development of cognitive function in infants through direct interaction with these receptors. the result of this study showed that the full-length sheep lf had the highest binding energy (-1627.8 and - 1051.7 kcal/mol for lrp and intelectin receptors, respectively) among other studied lfs. the second highest binding energy belonged to goat lf (-1551.7 and -1001.4 kcal/mol for lrp and intelectin receptors, respectively) and the lowest energy belonged to horse lf (-1190.1 kcal/mol) and single-humped camel lf (-920.9 kcal/mol) for lrp and intelectin receptors, respectively.

Conclusion

In summary, this study was the first attempt to examine the ability of the binding of lactoferrin from different origin to receptors involved in development of cognitive in infants. the results showed the lf may effect on the development of cognitive function, constitute a promising approach for supplemental or sole source nutrition for infants. in addition, our results suggested that the sheep lactoferrin is more effective than other lfs. it is also clear that the action of the sheep lf and its lobes on the cognitive function cannot be completely understood without experimental evidence.

Keywords

Lactoferrin, in silico, brain, cognitive function, infants