Reinaldo Barros Geraldo, J Stem Cell Res Ther 2014, 4:9
http://dx.doi.org/10.4172/2157-7633.S1.007

OMICS Group Conferences
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3rd International Conference and Exhibition on
Cell & Gene Therapy
October 27-29, 2014 Embassy Suites Las Vegas, USA

Looking for β3 integrin family selectivity: The use of snake venom disintegrin as a tool for molecular modeling approach

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Disintegrins are a family of modulatory peptides that inhibit the some integrins, such as αIIbβ3, αvβ3 and α5β1, which are involved in a variety of cellular functions such as platelet aggregation and angiogenesis, physiopathology of arterial thrombosis and cancer. These disintegrins were identified several sources including venom of some snakes. The aims of this study were to analyze using in silico approaches (i.e. molecular modeling and molecular dynamics) this disintegrin sub-family, to observe the selectivity against those integrins. And also perform a study of molecular biology with two disintegrins present in the venom of *Bothrops jararaca* venom, jararacin and jarastatin, to use these disintegrins as a model for study of new prototype of new drugs against those pathologies. The *in silico* analyses of 70 snake venoms disintegrins showed with the alignment and phylogeny results, the presence of four distinct sub-groups that posses the high similarity among them. From those subgroups, we select two disintegrins of these four sub-groups: Sub-group 1(albolatin and mojastin), sub-group 2 (jarastatin and salmosin) sub-group 3 (trimestatin and flavoridin) group 4 (kistrin and jararacin), and whose were used to construct the complexes with integrins αIIbβ3, αvβ3 and α5β1. These complexes were minimized with the GROMACS program. And the interaction of them was analyzed with the webservers PISA, protein interaction calculator (PIC) and GROMACS program. The analysis of the complexes with α5β1, the sub-group 1 and sub-group 3 and kistrin present the number of interations is greater than others. The αIIbβ3 complexes show the jararacin, sub-group 1 and sub-group 3 present the number of interactions is greater than thesub-group 2 and kistrin. And the αvβ3 complexes show sub-group 2 with the high interactions values than others followed by sub-group 3 and sub-group 1. The molecular dynamics reveals corroborated the initial *in silico* results that shows jararacin to αIIbβ3 complex formation and jarastatin posses more stability of αvβ3 complex formation. This study shows the presence of subgroups in the PII-disintegrins, and they present a different selectivity against integrins. And we succeeded in producing recombinant disintegrins of Bothrops jararaca with the maintenance of biologicalactivity.

Biography

Reinaldo Barros Geraldo is a young Scientist, Researcher currently Post-doc at Fluminense Federal University (Brazil). He graduated in Biomedicine Fluminense Federal University (2007), Master of Neuroimmunology, Fluminense Federal University (2009) and Doctor of Science by Federal University of Rio de Janeiro (2013). He has experience in the areas of biochemistry, with an emphasis on computer modeling, acting on the following subjects: Comparative modeling, structural biochemistry and Molecular Biology. Till now, he has published 11 papers in reputed journals.

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