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ISCB LATIN AMERICA BIOINFORMATICS CONFERENCE 2016

BUENOS AIRES ARGENTINA

NOVEMBER 21-23

CONFERENCE PROGRAM

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ISCB INTERNATIONAL SOCIETY FOR COMPUTATIONAL BIOLOGY

Phylogenetic and molecular docking analysis of conglutin γ from *Lupinus albus* reveals interaction with human insulin receptor

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Background: Conglutin γ is a protein with anti-hyperglycemic activity on rats and cell cultures and is suitable for type-II diabetes treatment. It binds to human insulin, but there is no information about its interaction with other medical important targets. For this reason, the present work reports a phylogenetic study of conglutin γ from *L. albus* and evaluates its interaction with known molecules that controls glycemia using molecular docking.

Results: Protein sequences with 20-80% amino acid conservation with conglutin γ were obtained from GenBank. Substitution models and tridimensional structure prediction were obtained using ModelGenerator and Phyre2, using monomeric form of conglutin γ. Maximum likelihood phylogeny was constructed using PHYML, which shows that amino acid sequence of conglutin γ is grouped with 7S basic globulins from *Glicine max* and *Morus notabilis*. For molecular docking analysis with conglutin γ, PDB files of human insulin and different related molecules (insulin-like growth factor I and II, human insulin receptor) were downloaded, refined with 3DRefine and prepared using Chimera. Molecular docking was performed on ClusPro and minimum energy of the best models selected by CONSRANK was compared. This simulation shows a highly notable binding prediction value only with human insulin receptor.

Conclusions: Conglutin γ from *Lupinus albus* is a protein with low conservation of amino acids outside the lupin group, and its monomeric form shows a high probability of interaction with human insulin receptor. This is an extra evidence for its insulin-mimetic action which re-inforce its use in co-treatment with metformin.

Supported by: UNMSM-VRIP (Código: 161005GE).