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In silico, in vitro and cytotoxicity investigations of biphenylalanine and its derivatives as potential HIV-1 gp120 attachment inhibitors

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In this study, molecular modeling and docking of gp120-CD4 protein complex crystal structure (PDBID: 1g9n) was used to design a novel attachment inhibitor, biphenylalanine and its derivatives (BPAs) that target HIV-1 gp120 and prevent its binding to CD4 on host cell. Molecular docking results by AutoDock Vina showed that L-biphenylalanine has highest binding probability than D-biphenylalanine and L-methyl-biphenylalanine and exhibited low negative docked energy. The CD4 capture ELISA experiments indicated that L-biphenylalanine has an IC_{50} at 200 μM. BPAs were non-toxic up to 400 μM in the Vero cell cytotoxicity test. In addition, BPAs fulfill "the Lipinski rule of five" criteria as good drug candidates.

Biography

Teow Chong Teoh is currently a Senior Lecturer of Bioinformatics program, Institute of Biological Sciences, Faculty of Science, Malaysia. He has obtained his BSc and MSc degrees in Biochemistry and PhD degree in Computational Chemistry from University of Malaya. He has 10 years of research experience in molecular modeling and simulation for chemical and biological systems. He has published numerous ISI/WOS journals, presented research papers in conferences and is holding the Chinese and US patents and has reviewed a number of research manuscripts. He has received research grants from University of Malaya and Malaysian Government for his research projects. He is also the Secretary of Malaysian Society of Marine Sciences.

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