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Exploration of substrate binding mode on n-terminal region of HIV-1 glycoprotein 41

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HIV (Human Immunodeficiency Virus), weakens the human immune system and keeps the body vulnerable to disease. There are many drugs having anti-HIV properties. They can be used in single or combination forms. Although drug combinations are meaningful way to slow down the disease progression of AIDS but there are no drugs that completely eliminate this disease. Also these drugs have some disadvantages: Viral resistances, adverse effects and high cost. We were interested in HIV target, Glycoprotein 41(gp 41). Gp41 is an envelope protein of HIV and has an important role in HIV entry. The gp 41 facilitates bounding HIV to cell surface receptors. There is no x-ray structure of full length of gp 41(345 a.a). X-ray structures of gp41 deposited in protein data bank belonging to synthetic C-peptides and N-peptides derived from the NHR and CHR regions of gp41. T-20(Enfuvirtide/Fuzeon) is the first drug approved in 2003 for gp41. It contains 36 residue derived from CHR region of gp41. Application of this drug T-20 is limited due to the high production of cost of the peptide and lack of its oral availability. Therefore, it is highly desirable developing new inhibitors. The N-terminal region has highly conserved hydrophobic grooves having deep hydrophobic pocket key point to stabilize of the six-helical bundle and viral entry. Eventually, the hydrophobic pocket of N-terminal peptide is a potential drug target of gp 41. For the HIV target gp41, interaction of the promising ligand A12 with monomer, trimer, and pentamer forms of N-terminal region of gp41 was studied using AutoDock Vina program to explore binding mode. Calculations were done for the structures of gp41 NHR monomer is 2zzo, NHR trimer, 2q7c, 2r5d and 1aik and NHR pentamer 1aik. Our quantitative results and visiual inspection show that the 1aik pentamer structure is the most appropriate structure for molecular docking. In the second part of the study for gp41, virtual ligand screening was done for the subset obtained from ZINC database to find out new, and small potential inhibitors. The results obtained from these studies will contribute both to the design and synthesis of some new and potent inhibitor candidates for HIV target gp41.

Biography

Vildan Adar has completed his PhD in 1997 from Hacettepe University and postdoctoral studies from UCLA, Department of Chemistry and Biochemistry (2001-2004), University of Cambridge, Unilever Centre for Molecular Science Informatics (2005) and University of Edinburgh, School of Biological Sciences, Institute of Structural & Molecular Biology (2006). She is Full Professor at Hacettepe University since 2006. She has published peer-reviewed research and review articles; and presented her research works in several international prestigious conferences and congresses. One of her papers at *J. Phys. Chem. A* (2003) was cited around 190 times by other researchers. Her research interests are computer-aided drug design, theoretical studies on organic reaction mechanism, and organic synthesis. Currently her research group works on following topics; Anti-AIDS drugs, Anticoagulant drugs, Anti-smoking drugs and MAO-A inhibitors.

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