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In Silico screening for anti-HPV agents using docking studies

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Abstract

HPV (Human PapillomaVirus) is known as one of the papillomavirus family which is able to infect humans. For more than 90% of cervical cancer, especially squamous cell carcinoma, HPV infection appears to be a necessary factor. Although HPV vaccination was recommended in almost all developed countries, including JAPAN, very recently, serious adverse events were reported. Thus, anti-HPV agents should be developed in order to prevent many types of cervical cancers. However, since more than 120 types of HPVs have been identified, it is not easy to inhibit the tumor promoting activities of all carcinogenic HPVs.

In this study, we tried to develop HPV E6 protein inhibitors using *in Silico* screening, especially, docking studies. The obtained agents are not for anti-cancer drugs but for in vitro studies which can reveal whether E6 protein inhibitors are capable of suppressing canceration of HPV infected cells. If the inhibitors have such activities, it is not impossible to develop anti-HPV drugs for almost all types of carcinogenic HPVs. We applied two kinds of methods: one is an ordinal *in Silico* screening using docking studies, and the other is a pharmacophorescreening plus docking studies using the co-crystal structure of HPV E6 protein and PDZ domain. We obtained some lead chemical structures, which are appeared to be effective for revealing the mechanism of canceration of HPV infected cells, using above two kinds of methods.

Biography

Tatsuya TAKAGI has completed his Ph.D at the age of 32 years from Osaka University. At that time, he had been a research assistant (this position corresponds to Assistant Professor in the USA) of School of Pharmaceutical Sciences, Osaka University for 5 years. Then, since 1993, he had worked for the Genome Information Research Center, Osaka University as a lecturer (this position corresponds to Associate Professor in the USA) until he became a professor of Graduate School of Pharmaceutical Sciences, Osaka University in 1998.He has published more than 100 papers in reputed journals and serving as avice deputy chairman of Division of Structure-Activity Relationship of the Pharmaceutical Society of Japan.