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In silico screening for anti-HPV agents using pharmacophore models

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HPV (Human Papillomavirus) is known as one of the papillomavirus family which is able to infect humans. HPV infection appears to be a necessary prerequisite for more than 90% of cervical cancer, especially squamous cell carcinoma. 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. Last year, at this conference, the author reported some candidate compounds which can be HPV E6 protein inhibitors developed by using *in silico* screening, especially, docking studies. However, 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. Thus, in this study the author tried to develop other candidates of HPV E6 protein inhibitors which can be more drug-like using *in silico* drug-like compounds database. Some lead chemical structures, which appeared to be effective not only for revealing the mechanism of canceration of HPV infected cells, but also for some key compounds of anti-HPV E6 inhibitors were obtained.

Biography

Tatsuya Takagi completed his PhD at the age of 32 from Osaka University. He was an Assistant Professor 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 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 is serving as Chairman of Division of Structure-Activity Relationship of the Pharmaceutical Society of Japan.

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