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Screening novel HIV-1 inhibitors targeting cyclophilin A by structure-based and ligand-based *in silico* study

Since cyclophilin A has peptidyl-prolyl isomerase activity and binds to the capsid protein of *Human Immunodeficiency Virus* (HIV), it is an attractive target as an anti-HIV drug. However, just a few drugs against HIV-1 infection targeting cyclophilin A has been developed and none of them has been approved. We found a number of active compounds by *in silico* structure-based screenings applying to the database with 1, 300 compounds recently. Although we found three docking sites A, B, and C, using MOE alpha site finder module, we used all of them as the docking sites because the three pockets were small. Two compounds, 12 and 23, were obtained as the most active ones. 12 covered the two docking sites, B and C, by cation-π interactions while the other covered B and C by CH-π and hydrogen bond. Especially, both of them exhibited anti-HIV activity against viral replication at low concentrations and relatively low cytotoxicity at the effective concentrations inhibiting viral growth by 50 %. As the results of comparisons between the obtained two compounds and the two controls which was called D4 and FD8, our compounds showed better results.

Biography

Tatsuya Takagi has completed his PhD from Osaka University. At that time, he had been 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 an Associate Professor 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 Chairman of Division of Structure-Activity Relationship of the Pharmaceutical Society of Japan.

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