Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Design of new inhibitors for H5N1 avian influenza using a molecular dynamics simulation JIN WOO PARK, WON HO JO, Seoul National University — Recently, there has been a growing interest in the treatment of H5N1 avian influenza. One of the most widely used antiviral agents is oseltamivir. However, it has been reported that oseltamivir is not as effective against the neuraminidase subtype N1 as it is against subtypes N2 and N9. In our research we addressed this problem by designing new inhibitors and these altered inhibitor's binding affinities were calculated. In this study, we introduced chemical groups to the existing oseltamivir, so to fit into the newly discovered cavity in the subtype N1. When the binding strengths of the oseltamivir and the newly designed inhibitors for N1 were calculated to examine the drug efficiency through a molecular dynamics simulation, then compared with each other, it was found that one of the designed molecules exhibited a strong binding affinity, with more than twice the binding strength than that of oseltamivir. Since the aforementioned designed inhibitor appears to have the possibility for oral activity according to the criteria of human oral bioavailability, we propose that the inhibitor is a promising antiviral drug for H5N1 avian influenza.

Jin Woo Park
Seoul National University

Date submitted: 27 Nov 2007 Electronic form version 1.4