

CONFORMATIONAL STUDIES OF THE HUMANIZED HBV PRE-S2 ANTIBODY AND ITS DOCKING TO HBV ANTIGEN *ADR*

Ky Youb Nam, Hyo Jeong Hong*, Seung-Moak Kim*, Kyoung Tai No
Department of Chemistry, Soong Sil University

*Korea Reserch Institute of Bioscience and Biotechnology

Molecular docking studies were performed for a humanized HBV Pre-S2 antibody and its antigen *adr*. Antigen structure was taken from NMR experiment and antibody structure was determined by using homology technique. At first step, Grid search was performed for finding energetically favorable orientations antigen. Next step, Since the entrance of their binding pocket formed by the CDRs of the model antibody is narrow, the CDRs conformations of the model antibody is changed to those of 1ggi antibody-antigen complex which were observed by x-ray crystallography. The same method was used for finding suitable orientation and minima. This systematic approach may lead to find the orientation and site of bound antigen binding and will apply to antibody design. Our work followed the idea of *induced fit* mechanism.