

參考文獻

Abagyan, R., and Totrov, M. (2001). High-throughput docking for lead generation. *Curr. Opin. Chem. Biol.* 5:375 - 382.

Aloy, P., Querol, E., Aviles, F.X., and Sternberg, M.J.E. (2001). Automated Structure-based prediction of functional site in proteins: application to assessing the validity of Inheriting protein function from homology in genome annotation and to protein docking. *J. Mol. Biol.* 311:395-408.

Bazan, J.F., and Fletterick, R.J. (1990). Structural and catalytic models of trypsin-like viral proteases. *Semin. Virol.* 1:311-322.

Brinkworth, R. I., Fairlie, D.P., Leung, D., and Young, P.R. (1999). Homology model of the dengue 2 virus NS3 protease : putative interactions with both substrate and NS2B cofactor. *J. Gen. Virol.* 80:1167 - 1177.

Cecconi, F., Micheletti, C., Carloni, P., and Maritan, A. (2001). Molecular dynamics studies on HIV-1 protease drug resistance and folding pathways. *Proteins.* 43:365-372.

Chen, B., Piletsky, S., and Turner, A.P.F. (2002). High molecular recognition: design of "Keys". *Comb Chem High T. Scr.* 5(6):409-427.

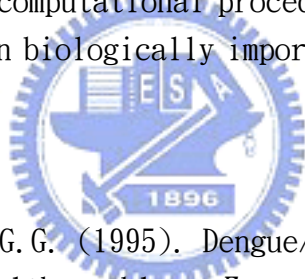
Clark, R.D., Strizhev, A., Leonard J.M., Blake, J.F., and Matthew, J.B. (2002). Consensus scoring for ligand/protein interactions. *J. Mol. Graphics Mod.* 20:281 - 295.

Eldridge, M. D., Murray, C. W., Auton, T. R., Paolini, G. V., and Mee, R. P. (1997). Empirical scoring functions: I. The development of a fast empirical scoring function to estimate the binding affinity of ligands in receptor complexes. *J. Comput. Aided. Mol. Des.* 11(5):425-445.

Falgout, B., Pethel, M., Zhang, Y-M., Lai, C-J. (1991). Both nonstructural proteins NS2B and NS3 are required for the proteolytic processing of dengue virus nonstructural proteins. *J. Virol.* 65:2467-2475.

Freceer, V., Kabelac, M., De Nardi, P., Pricl, S., and Miertus, S. (2004). Structure-based design of inhibitors of NS3 serine protease of hepatitis C virus. *J. Mol. Graphics Mod.* 22:209 - 220.

Goodford, P. J. (1985). A computational procedure for determining energetically favorable binding sites on biologically important macromolecules. *J. Med. Chem.* 28(7):849-857.



Gubler, D. J., and Clark, G. G. (1995). Dengue/dengue hemorrhagic fever : the emergence of a global health problem. *Emerg. Infect. Dis.* 1(2):55-57.

Guex, N., and Putsch, M. C. (1997). SWISS-MODEL and the Swiss - Pdb Viewer: An environment for comparative protein modeling. *Electrophoresis.* 18(15): 2714-2723.

Heinz, F. X., and Allison, S. L. (2001). The machinery for flavivirus fusion with host cell membranes. *Curr. Opin. Microbiol.* 4(4):450 - 455.

Henchal, E. A., and Putnak, J. R. (1990). The dengue virus. *Clin. Micro. Rev.* 3:376-396.

Hendlich, M., Rippmann, F., and Barnickel, G. (1997). LIGSITE: Automatic and efficient detection of potential small molecule-binding sites in proteins. *J. Mol. Graph. Model.* 15(6):359–363.

Joseph-McCarthy, D. (1999). Computational approaches to structure-base ligand design. *Pharmacol. Ther.* 84:179–191.

Kapoor, M., Zhang, L., Ramachandra, M., Kusukawa, J., Ebner K.E., and Padmanabhan, R. (1995). Association between NS3 and NS5 proteins of dengue virus type 2 in the putative RNA replicase is linked to differential phosphorylation of NS5. *J. Biol. Chem.* 270:19100–19106.

Kautner, I., Robinson, M. J., and Kuhnle, U. (1997). Dengue virus infection: epidemiology, pathogenesis, clinical presentation, diagnosis, and prevention. *J. Pediatr.* 131(4):516–524.

Kuhn, R. J., Zhang, W., Rossmann, M.G., Pletnet, S.V., Corver, J., Lenches, E., Jones, C.T., Mukhopadhyay S., Chipman, P.R., Strauss, E.G., Baker T.S., and Strauss, J.H. (2002). Structure of dengue virus: implications for flavivirus organization, maturation, and fusion. *Cell.* 108:717–725.

Li, H., Clum, S., You, S., Ebner K.E., and Padmanabhan, R. (1999). The serine protease and RNA-stimulated nucleoside triphosphatase and RNA helicase functional domains of Dengue virus type 2 NS3 coverge within a region of 20 amino acids. *J. Virol.* 73 (4):3108–3116.

Love, R. A., Parge, H.E., Wickersham, J.A., Hostomsky, Z., Habuka, N., Moomaw, E.W., Adachi, T., and Hostomska, Z. (1996). The crystal structure of hepatitis C virus NS3 proteinase reveals a trypsin-like fold and a structural zinc binding site. *Cell.* 87:331–342.

Mackenzie, J.M., Jones, M.K. and Young, P.R. (1996). Immunolocalization of the dengue virus nonstructural glycoprotein NS1 suggests a role in viral RNA replication. *Virology*. 220(1):232-240.

Matusan, A.E., Kelly, P.G., Pryor, M.J., Whisstock, J.C., Davidson, A.D., and Wright, P.J. (2001). Mutagenesis of the dengue virus type 2 NS3 proteinase and the production of growth-restricted virus. *J. Gen. Virol.* 82:1647 - 1656.

McBride, W.J., and Bielefeldt-Ohmann, H. (2000). Dengue viral infections: pathogenesis and epidemiology. *Microbes Infect.* 2:1041-1050.

Miranker, A., and Karplus, M. (1991). Functionality maps of binding sites: a multiple copy simultaneous search method. *Proteins*. 11(1):29-34.

Murthy, H.M.K., Clum, S., and Padmanabhan, R. (1999). Dengue virus NS3 serine protease. *J. Biol. Chem.* 274:5573-5580.



Murthy, H.M.K., Judge, K., DeLucas, L., and Padmanabhan, R. (2000). Crystal structure of dengue virus NS3 protease in complex with a Bowman-Birk Inhibitor: implications for flaviviral polyprotein processing and drug design. *J. Mol. Biol.* 301:759-767.

Schneider, G., and Böhm, H-J. (2002). Virtual screening and fast automated docking methods. *DDT*. 7:64-70.

Shoichet, B.K., McGovern, S.L., Wei, B., and Irwin, J.J. (2002). Lead discovery using molecular docking. *Curr. Opin. Chem. Bio.* 6:439-446.

Sternberg, M. J. E., Gabb, H. A., and Jackson, R. M. (1998). Predictive docking of protein-protein and protein-DNA complexes. *Curr. Opin. Struct. Biol.* 8: 250-256.

Valle, R. P. C., and Falgout, B. (1998). Mutagenesis of the NS3 protease of dengue virus type 2. *J. Virol.* 72(1):624-632.

Yusof, R., Clum, S., Wetzel, M., Murthy, H. M. K., and Padmanabhan, R. (2000). Purified NS2B/NS3 serine protease of dengue type 2 exhibits cofactor NS2B dependence for cleavage of substrate with dibasic amino acid in vitro. *J. Bio. Chem.* 275:9963-9969.

Zhang, L., Mohan, P. M., and Padmanabhan, R. (1992). Processing and localization of dengue virus type 2 polyprotein precursor NS3-NS4A-NS4B-NS5. *J. Virol.* 66:7549-7554.



王正雄，陳秀玲。氣候溫暖化對台灣登革熱流行之影響。中華衛誌。1997；16(6)：455-465。

吳盈昌。1981年屏東縣琉球鄉之第二型登革熱流行。中華微免雜誌。1986；19：203。

戴佛香。登革熱病毒與其感染。國防醫學雜誌。1991；13(6)：590-598。

杜武俊。登革熱病媒蚊。科學月刊。1995；26(11)：911-917。

莊榮輝。生物化學基礎。2000