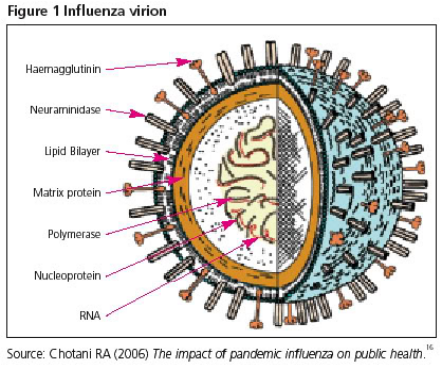
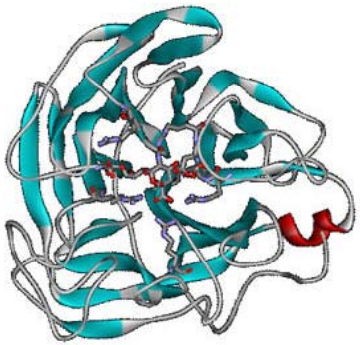
Joint International Tropical Medicine Meeting 2010 and the International Malaria Colloquium 2010

Application of bioinformatic tools: structural modeling and simulation of influenza viral proteins





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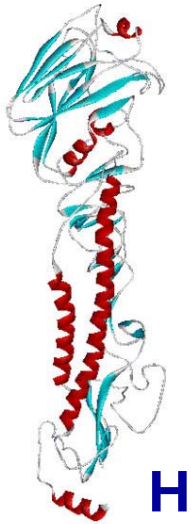

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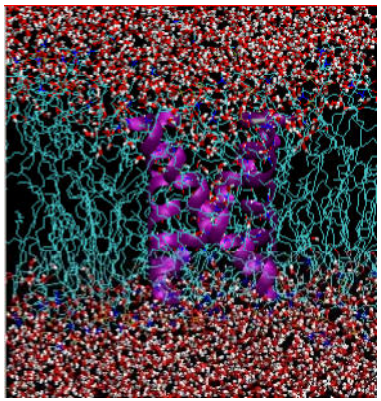

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Pornthep Sompornpisut

Computational Chemistry Unit Cell
Department of Chemistry,
Faculty of Science,
Chulalongkorn University, Bangkok,
Thailand.
E-mail: spornthe@hotmail.com

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Conclusions

- A general view on concepts of computational-aided molecular design approaches along with its applications in our research works on influenza viral proteins was presented.

- Homology modeling, molecular dynamics simulations, substrate binding free energy calculation and molecular docking techniques were employed to study:

  - Activation mechanism of hemagglutinin
  - Drug blockade of the H+ transport in M2 ion channel
  - Virtual screening of neuraminidase inhibitor from natural product compound library

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