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APPENDICES

1. Publication for this thesis

- 1.1 Nunthaboot, N., Tonmunpheap, S., Parasuk, V., Wolschann, P., Kokpol, S. Three-Dimensional Quantitative Structure Activity Relationships Studies on Diverse Structural Classes of HIV-1 Integrase Inhibitors using CoMFA and CoMSIA. *Eur. J. Med. Chem.* 41 (2006): 1359-1372.
- 1.2 Nunthaboot, N., Pianwanit, S., Parasuk, V., Kokpol, S., Briggs, J. M. Computational studies of HIV-1 integrase and its inhibitors. *Curr. Com. Aid. Drug. Des.* accepted.
- 1.3 Nunthaboot, N., Pianwanit, S., Parasuk, V., Ebalunode, J. O., Briggs, J. M., Kokpol, S. Hybrid Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulations of HIV-1 Integrase/Inhibitor Complexes. *Biophys. J.*, accepted after minor revision.
- 1.4 Nunthaboot, N., Pianwanit, S., Parasuk, V., Kokpol, S., Wolschann, P. Theoretical Study of HIV-1 Integrase Inhibition. *J. Mol. Struct. (Theochem)*, revised.

2. Publication for related work

- 2.1 Abd-Elazem, I. S., Nunthaboot, N., Kokpol, S., Pianwanit, S., Huang, R. C. C. Lithospermic acid and lithospermic acid B act at the active site of integrase to inhibit replication of human immunodeficiency virus type I. (2006). *J. Virol.* Submitted.

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1. **Nunthaboot, N.**, Tonmunphean, S., Parasuk, V., Wolschann, P., Kokpol, S. *Eur. J. Med. Chem.* 41 (2006): 1359-1372.
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3. **Nunthaboot, N.**, Pianwanit, S., Parasuk, V., Ebalunode, J. O., Briggs, J. M., Kokpol, S. *Biophys. J.*, accepted after minor revision.
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