Assist. Prof. Dr. Nadtanet Nunthaboot

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AREA OF INTERESTS

- Quantum Chemistry and QM/MM Calculations
- Molecular Dynamics Simulation
- Binding Free Energy Calculation using MM-PB(GB)SA method
- Computer Aided Molecular (Drug) Design
- Bioinformatics

COMPUTATIONAL SKILLS

- Computational Chemistry, Molecular Modeling and Drug Design software packages such as Gaussian, MOPAC, GAMESS, CHARMM, AMBER, SYBYL, Insight II, Autodock, DRAGON, MOE
- Unix and Windows operating system

INTERNATIONAL CONFERENCES

1. Quantitative Structure Activity Relationships Studies on HIV-1 Integrase Inhibitors using CoMFA and CoMSIA, The QSAR EURO, Istanbul, Turkey, 2004.
2. 3D-QSAR CoMFA and CoMSIA on HIV-1 Integrase inhibitors, Joint Meeting of the Austrian, Czech and German Pharmaceutical Societies, Regensburg, Germany, 2004.
3. Conformation of Derivatives of 4-Aryl-2, 4-dioxobutanoic acid: A Class of HIV-1 Integrase inhibitor, The 2nd Asian Pacific Conference on Theoretical & Computational Chemistry (APCTCC), Bangkok, Thailand, 2005.
4. CoMFA and CoMSIA 3D-QSAR study of HIV-1 Integrase Inhibitors, The 2nd Asian Pacific Conference on Theoretical & Computational Chemistry (APCTCC), Bangkok, Thailand, 2005.

5. Investigation of metal dependent behavior of HIV-1 integrase inhibitors: DFT calculation, American Chemical Society National Meeting, Atlanta, Georgia, USA, 2006.

6. Comparison of QM/MM and MM Force Fields in MD simulations of HIV-1 Integrase-5CITEP System. American Chemical Society Western Regional Meeting 2007 Frontiers in Chemistry, Biopharmaceuticals & Biotechnology. San Diego, CA, USA. 2007.

7. Computer-Aided Drug Design of HIV-1 Integrase Inhibitors: Three-Dimensional Quantitative Structure Activity Relationship Study, Molecular Design and Computer-assisted Combinatorial Chemistry, Trieste, Italy. 2008.

8. Dynamics of Photoinduced Charge Transfer Interaction in FMN binding Protein. Pure and Applied Chemistry International Conference. Department of Chemistry, Faculty of Science, Naresuan University. 2009.

9. Correlation between Photoinduced Electron Transfer Rate and Structural Factors in FMN Binding Protein. Pure and Applied Chemistry International Conference. Department of Chemistry, Faculty of Science, Naresuan University. 2009.

10. Effects of Residues Changes on Human Receptor Binding Affinity of H1N1 Hemagglutinins: Insights from Molecular Dynamics Simulation. 14th International Annual Symposium on Computational Science and Engineering (ANSCSE 14). Mae Fah Luang University**.** Chiang Rai. 2010

11. Changes of human receptor binding affinity of H1N1 hemagglutinins: Insights from molecular dynamics simulation. 240th American Chemical Society National Meeting. Boston, MA, USA, 2010.

12. Comparison of the monomer structure of the FMN binding protein from Desulfovibrio vulgaris obtained by NMR and molecular dynamics simulation approaches. The VIIIth Congress of International Society of Theoretical Chemical Physics" (ISTCP-VIII). Budapest, Hungary, 2013.

NATIONAL CONFERENCES

1. Potential Energy Surface Studies of 4 – aryl - 2, 4 - dioxobutanoic acid compounds, The 29th Conference of Science and Technology of Thailand (STT29), Khon Kaen, Thailand, 2002.

2. Three-Dimensional Quantitative Structure-Activity Relationship (3D-QSAR) Studies of HIV-1 Integrase Inhibitors, The RGJ-PhD. VI Congress, Chonburi, Thailand, 2005.

3. Comparative molecular field analysis and comparative molecular similarity indices analysis of HIV-1 integrase inhibitors, The 9th Annual National Symposium on Computational Science and Engineering (ANSCSE 9), Bangkok, Thailand. 2005.

4. Docking calculations on HIV-1 integrase inhibitors: insight in to the binding modes of diketo acids, The 31st Conference of Science and Technology of Thailand (STT31), Nakorn Ratchasrima, Thailand, 2005.

5. A QSAR study of diverse structural classes of HIV-1 Integrase Inhibitors, Thai-Austria Theoretical Chemistry Collaboration: A Successful Interdisciplinary Cooperation, Bangkok, Thailand, 2006.

6. Binding Interaction between HIV-1 Integrase and Lithospermic Acid: A Computational Docking Study, The 11th Annual National Symposium on Computational Science and Engineering (ANSCSE 11), Prince of Songkla University, Phuket campus, Phuket, Thailand. 2007.

7. Insight into Specific Binding of Hemagglutinin with SA-alpha-2,3-Gal and SA-alpha-2,6-Gal: QM/MM MD Simulations, Global Concerns, Recent Outbreak and Molecular Insight into Avian Influenza H5N1, Bangkok, Thailand, 2008.

8. Molecular insights of human receptor binding to 2009 H1N1 influenza A hemagglutinin. Holiday Inn, Hua Hin, Thailand 2009.

9. Evolution of Human Receptor Binding Affinity of H1N1 Hemagglutinins from 1918 to 2009 Pandemic Influenza A Virus: Insights from molecular dynamics simulation. Holiday Inn, Hua Hin, Thailand 2010.

10. Electronic absorption and vertical excitation energies of flavin containing BLUF protein. The 8th-Thai Summer School of Computational Chemistry “Excited-state calculation in chemical and biological systems” Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang mai, Thailand, September 24-27, 2011

PUBLICATIONS

1**. Nadtanet Nunthaboot**, Somsak Tonmunphean, Vudhichai Parasuk, Peter Wolschann, and Sirirat Kokpol. Three-Dimensional Quantitative Structure Activity Relationships Studies on Diverse Structural Classes of HIV-1 Integrase Inhibitors using CoMFA and CoMSIA. *European Journal of Medicinal Chemistry*. 41, 1359-1372, 2006.

2. **Nadtanet Nunthaboot**, Somsak Pianwanit, Vudhichai Parasuk, Sirirat Kokpol, and James M. Briggs. Computational studies of HIV-1 integrase and its inhibitors. *Current Computer-Aided Drug Design.* 3, 160-190, 2007.

3. **Nadtanet Nunthaboot**, Somsak Painwanit, Vudhichai Parasuk, Sirirat Kokpol, and Peter Wolschann. Theoretical study on the HIV-1 integrase inhibitor 1-(5-chloroindol-3-yl)-3-hydroxy-3-(2H-tetrazol-5-yl)-propenone (5CITEP). *Journal of Molecular Structure*. 844-845, 208-214, 2007.

4. **Nadtanet Nunthaboot**, Jerry O. Ebalunode, Somsak Painwanit, Vudhichai Parasuk, James M. Briggs and Sirirat Kokpol. Hybrid Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulations of HIV-1 Integrase/Inhibitor Complexes. *Biophysical Journal*. 93, 3613-3626, 2007.

5. **Nadtanet Nunthaboot**, Fumio Tanaka, Sirirat Kokpol, Haik Chosrowjan, Seiji Taniguchi, and Noboru Mataga. Simultaneous Analysis of Ultrafast Fluorescence Decays of FMN Binding Protein and Its Mutated Proteins by Molecular Dynamic Simulation and Electron Transfer Theory. *Journal of Physical Chemistry B.* 112, 13121-13127, 2008.

6. **Nadtanet Nunthaboot**, Fumio Tanaka, Sirirat Kokpol, Haik Chosrowjan, Seiji Taniguchi, Noboru Mataga. Quantum Mechanical Study of Photoinduced Charge Transfer in FMN Binding Protein. *Journal of Physical Chemistry B.*112, 15837-15843, 2008.

7. **Nadtanet Nunthaboot**, Fumio Tanaka, Sirirat Kokpol, Haik Chosrowjan, Seiji Taniguchi, Noboru Mataga. Simulation of ultrafast non-exponential fluorescence decay induced by electron transfer in FMN binding protein. *Journal of Photochemistry and Photobiology A: Chemistry*. 201, 191-196, 2008.

8. Thanyada Rungrotmongkol, Panita Decha, Pornthep Sompornpisut, Maturos Malaisree, Pathumwadee Intharathep, **Nadtanet Nunthaboot**, Thanyarat Udommaneethanakit, Ornjira Aruksakunwong, Supot Hannongbua. Combined QM/MM mechanistic study of the acylation

process in furin complexed with the H5N1 avian influenza virus hemagglutinin's cleavage site. *Proteins*. 76, 62-71, 2008.

9. Maturos Malaisree, Thanyada Rungrotmongkol, **Nadtanet Nunthaboot**, Ornjira Aruksakunwong, Pathumwadee Intharathep, Panita Decha, Pornthep Sompornpisut, Supot Hannongbua. Source of Oseltamivir Resistance in Avian Influenza H5N1 Viruses with the H274Y Mutation. *Amino Acids*. *37*, 725-732, 2009.

10. Thanyada Rungrotmongkol, Pathumwadee Intharathep, Maturos Malaisree, **Nadtanet Nunthaboot**, Nopphorn Kaiyawet, Pornthep Sompornpisut, Sanchai Payungporn, Yong Poovorawan and Supot Hannongbua. Susceptibility of antiviral drugs against 2009 influenza A (H1N1) virus. *Biochemical and Biophysical Research Communications. 385*, 390-394, 2009.

11. Banchob Wanno, Wandee Rakrai, Somchai Keawwangchai, Neramit Morakot, Nongnit Morakot, **Nadtanet Nunthaboot**, Vithaya Ruangpornvisuti. A density functional investigation of 1,3-bis(4-nitrophenyl)urea as anion receptor. J*ournal of Molecular Structure: THEOCHEM*. *902*, 33-40, 2009.

12. **Nadtanet Nunthaboot,** Fumio Tanaka, Sirirat Kokpol. Analysis of Photoinduced Electron Transfer in AppA. *Journal of Photochemistry and Photobiology A: Chemistry. 207*, 274-281, 2009.

13. Thanyada Rungrotmongkol, Thanyarat Udommaneethanakit, Maturos Malaisree, **Nadtanet Nunthaboot**, Pathumwadee Intharathep, Pornthep Sompornpisut and Supot Hannongbua. How does each substituent functional group of oseltamivir lose its activity against virulent H5N1 influenza mutants? *Biophysical Chemistry. 145*, 29-36, 2009.

14. Fumio Tanana and **Nadtanet Nunnthaboot**. Correlation between photoinduced electron transfer rate and structural factors in FMN binding protein. *Proceeding: Pure and Applied Chemistry International Conference*. 491-494, 2009.

15. **Nadtanet Nunnthaboot** and Fumio Tanana. Dynamic of photoinduced charge transfer interaction in FMN binding protein. *Proceeding: Pure and Applied Chemistry International Conference*. 495-499, 2009.

16. Thanyada Rungrotmongkol, Maturos Malaisree, **Nadtanet Nunthaboot**, Pornthep Sompornpisut, and Supot Hannongbua. Molecular Prediction of Oseltamivir Efficiency

against Probable Influenza A (H1N1-2009) Mutants: Molecular Modelling Approach. *Amino Acids*. *39*, 393-398. 2010.

17. **Nadtanet Nunthaboot**, Thanyada Rungrotmongkol, Maturos Malaisree, Panita Decha, Nopphorn Kaiyawet, Pathumwadee Intharathep, Pornthep Sompornpisut, Yong Poovorawan and Supot Hannongbua. Molecular insights into human receptor binding to 2009 H1N1 influenza A hemagglutinin. *Monatshefte für Chemie. 141*, 801-807, 2010.

18. **Nadtanet Nunthaboot**, Thanyada Rungrotmongkol, Maturos Malaisree, Nopphorn Kaiyawet, Panita Decha, Pornthep Sompornpisut, Yong Poovorawan and Supot Hannongbua. Evolution of Human Receptor Binding Affinity of H1N1 Hemagglutinins from 1918 to 2009 Pandemic Influenza A Virus. *Journal of Chemical Information and Model*ing, *50*, 1410-1417, 2010.

19. **Nadtanet Nunthaboot**, Fumio Tanaka, Sirirat Kokpol. Simultaneous analysis of photoinduced electron transfer in wild type and mutated AppAs. *Journal of Photochemistry and Photobiology A: Chemistry*. *20*9, 79-87, 2010.

20. Rong Rujkorakarn, **Nadtanet Nunthaboot**, Fumio Tanaka, Pimchai Chaiyen, Haik Chosrowjan, Seiji Taniguchi, Noboru Mataga. Time-resolved Stokes shift in proteins with continuum model: Slow dynamics in proteins. *Journal of Photochemistry and Photobiology A: Chemistry*. *215*, 38-45, 2010.

21. Thanyada Rungrotmongkol, **Nadtanet Nunthaboot**, Maturos Malaisree, Nopporn Kaiyawet, Pathumwadee Yotmanee, Arthitaya Meeprasert and Supot Hannongbua**.** Molecular insight into the specific binding of ADP-ribose to the nsP3 macro domains of chikungunya and Venezuelan equine encephalitis viruses: molecular dynamics simulations and free energy calculations. *Journal of Molecular Graphics and Modelling*. 29, 347-353, 2010.

22. Pathumwadee Intharathep, Thanyada Rungrotmongkol, Panita Decha, **Nadtanet Nunthaboot**, Nopphorn Kaiyawet, Teerakiat Kerdcharoen, Pornthep Sompornpisut, Supot Hannongbua. Evaluating how rimantadines control the proton gating of the influenza A M2-proton port via allosteric binding outside of the M2-channel: MD simulations. *Journal of Enzyme Inhibition and Medicinal Chemistry*, 26, 162-168, 2011.

23.**Nadtanet Nunthaboot**, Somsak Pianwanit, Sirirat Kokpol and Fumio Tanaka. Simultaneous analyses of photoinduced electron transfer in the wild type and four single substitution isomers of the FMN binding protein from *Desulfovibrio vulgaris*, Miyazaki F. *Physical Chemistry Chemical Physics*. 13, 6085-6097, 2011.

24. Kiattisak Lugsanangarm, Somsak Pianwanit, Sirirat Kokpol, **Nadtanet Nunthaboot**, Haik Chosrowjan, Seiji Taniguchi, Fumio Tanaka. Theoretical analyses of photoinduced electron transfer in medium chain acyl-CoA dehydrogenase: Electron transfer in the normal region. *Journal of Photochemistry and Photobiology A: Chemistry. 224, 80-90, 2011.*

25. Thanyada Rungrotmongkol**,** Pathumwadee Yotmanee, **Nadtanet Nunthaboot,** Supot Hannongbua. Computational studies of influenza A virus at three important targets: hemagglutinin, neuraminidase and M2 protein. *Current Pharmaceutical Design*. *17,* 1720-1739, 2011.

26. Arthitaya Meeprasert, Wasinee Khuntawee, Kittiwat Kamlungsua, **Nadtanet Nunthaboot**, Thanyada Rungrotmongkol, Supot Hannongbua. Binding pattern of the long acting neuraminidase inhibitor laninamivir towards influenza A subtypes H5N1 and pandemic H1N1. Journal of Molecular Graphics and Modelling, 38, 148-154, 2012.

27. Chanukorn Tabtimsai, Somchai Keawwangchai, **Nadtanet Nunthaboot**, Vithaya Ruangpornvisuti, Banchob Wanno. Density functional investigation of hydrogen gas adsorption on Fe-doped pristine and Stone-Wales defected single-walled carbon nanotubes. Journal of Molecular Modeling. 18, 3941-3949, 2012.

28. Arthit Nueangaudom, Kiattisak Lugsanangarm, Somsak Pianwanit, Sirirat Kokpol, **Nadtanet Nunthaboot** and Fumio Tanaka. Structural basis for the temperature-induced transition of D-amino acid oxidase from pig kidney revealed by molecular dynamic simulation and photo-induced electron transfer. Phys. Chem. Chem. Phys. 14, 2567-2578, 2012.

29. Arthit Nueangaudom, Kiattisak Lugsanangarm, Somsak Pianwanit, Sirirat Kokpol, **Nadtanet Nunthaboot**, Fumio Tanaka The mechanism of photoinduced electron transfer in the d-amino acid oxidase–benzoate complex from pig kidney: Electron transfer in the inverted region. Journal of Photochemistry and PhotobiologyA: Chemistry, 250, 6-17, 2012.

30. **Nadtanet Nunthaboot**, Thanyada Rungrotmongkol, Ornjira Aruksakunwong and Supot Hannongbua. Effects of the protonation state of the catalytic residues and ligands upon binding and recognition in targeted proteins of HIV-1 and influenza viruses. Current Pharmaceutical Design. 19, 4276-4290, 2013.

31. **Nadtanet Nunthaboot**, Nobuo Kido, Fumio Tanaka, Kiattisak Lugsanangarm, Arthit Nueangaudom, Somsak Pianwanit, Sirirat Kokpol. Relationship between rate of photoinduced electron transfer and hydrogen bonding chain of tyrosine-glutamine-flavin in flavin photoreceptors: Global analyses among four TePixDs and three AppAs. Journal of Photochemistry and Photobiology A: Chemistry, 252, 14-24, 2013.

32. Kiattisak Lugsanangarm, Somsak Pianwanit, Arthit Nueangaudom, Sirirat Kokpol, Fumio Tanaka, **Nadtanet Nunthaboot**, Kumiko Ogino, Rikako Takagi, Takeshi Nakanishi, Masaya Kitamura, Seiji Taniguchi, Haik Chosrowjan. Mechanism of photoinduced electron transfer from tyrosine to the excited flavin in the flavodoxin from Helicobacter pylori. A comparative study with the flavodoxin and flavin mononucleotide binding protein from Desulfovibrio vulgaris (Miyazaki F) Journal of Photochemistry and Photobiology A: Chemistry, 268, 58-66, 2013.

33. **Nadtanet Nunthaboot**, Kiattisak Lugsanangarm, Arthit Nueangaudom, Somsak Pianwanit, Sirirat Kokpol, Fumio Tanaka. Photoinduced Electron Transfer Modeling to Simulate Flavoprotein Fluorescence Decay. Fluorescence Spectroscopy and Microscopy Methods in Molecular Biology. 1076, 337-355. 2014.

34. Arthit Nueangaudom, Kiattisak Lugsanangarm, Somsak Pianwanit, Sirirat Kokpol, **Nadtanet Nunthaboot** and Fumio Tanaka. Non-equivalent conformations of D-amino acid oxidase dimer from porcine kidney between the two subunits. Molecular dynamics simulation and photoinduced electron transfer. Phys. Chem. Chem. Phys.,16, 1930-1944, 2014.

35. **Nadtanet Nunthaboot,** Kiattisak Lugsanangarm, Somsak Pianwanit, Sirirat Kokpol, Fumio Tanaka, Seiji Taniguchi, Haik Chosrowjan, Takeshi Nakanishi, Masaya Kitamura. Bell-shaped dependence of the rate of ultrafast photoinduced electron transfer from aromatic amino acids to the excited flavin on the donor–acceptor distance in FMN binding proteins Computational and Theoretical Chemistry, 1030, 9-16, 2014.

36. **Nadtanet Nunthaboot**, Fumio Tanaka, Sirirat Kokpol Comparison of the monomer structure of the FMN-binding protein from Desulfovibrio vulgaris obtained by NMR and molecular dynamics simulation approaches. Molecular Simulation. 40, 1026-1034, 2014.

37. Kiattisak Lugsanangarm, Sirirat Kokpol, Arthit Nueangaudom, Somsak Pianwanit, **Nadtanet Nunthaboot** and Fumio Tanaka. Structural heterogeneity among four subunits in pyranose 2-oxidase: A molecular dynamics simulation study. Journal of Theoretical and Computational Chemistry **13**, 1440010-2014.

38. **Nadtanet Nunthaboot**, Fumio Tanaka, Sirirat Kokpol, Nina V. Visser, Herbert van Amerongen and Antonie J. W. G. Visser. Molecular dynamics simulation of energy migration between tryptophan residues in apoflavodoxin RSC Advances, 4, 31443-31451, 2014.

39. Arthit Nueangaudom, Kiattisak Lugsanangarm, Somsak Pianwanit, Sirirat Kokpol, **Nadtanet Nunthaboot**, Fumio Tanaka, Seiji Taniguchi[c] and Haik Chosrowjan. Theoretical analyses of the fluorescence lifetimes of the D-amino acid oxidase–benzoate complex dimer from porcine kidney: molecular dynamics simulation and photoinduced electron transfer. RSC Advances**,** 4, 54096-54108, 2014.