

August 4, 2010			
9.00-9.50	<p>Opening Ceremony <i>Place: Grand Ballroom (3rd floor)</i></p> <p>Professor Ahmad Ali Foroughi Abari, The President of Azad University, Khorasgan, Iran Assoc. Prof. Tutus Gusdinar Kartawinata, Dean of the School of Pharmacy, Bandung Institute of Technology, Indonesia</p> <p>Professor Dr. Pongsak Angkasith, President of Chiang Mai University, Thailand Progress Report By Dean of Faculty of Science, Chiang Mai University</p>		
9.50-10.40	<p>Plenary Lecture: “B_nN_n Nanomotor: A Novel Biomolecular Nanodetector” Prof. Dr. Majid Monajjemi <i>(Department of Chemistry, Science & Research Branch, Islamic Azad University, Tehran, Iran)</i></p> <p>Chair: Daryono Hadi Tjahjono</p>		
10.40-11.00	Break		
11.00-11.50	<p>Plenary Lecture: “Molecular Modeling on Viral Influenza A subtypes H5N1 and Pandemic H1N1” Prof. Dr. Supot Hannongbua <i>(Computational Chemistry Unit Cell, Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok, Thailand)</i></p>		
11.50-13.00	Lunch		
13.00-14.30	<table border="0" style="width: 100%;"> <tr> <td style="width: 50%; text-align: center;"> Executive Meeting Place: Chang Sean Room (3rd Floor) </td> <td style="width: 50%; text-align: center;"> Poster Session I Place: Grand Ballroom (3rd floor) </td> </tr> </table>	Executive Meeting Place: Chang Sean Room (3rd Floor)	Poster Session I Place: Grand Ballroom (3rd floor)
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Chair: Slamet Ibrahim			

14.30-15.00	<p style="text-align: center;">Place: Grand Ballroom (3rd floor)</p> <p style="text-align: center;">Invited Speaker: "Application of Computer in Pharmacokinetics"</p> <p style="text-align: center;">Prof. Dr. M. Hassanzadeh Khayyat</p> <p style="text-align: center;"><i>(Pharmaceutical Sciences Research Center, Department of Medicinal Chemistry, School of Pharmacy, Mashhad University of Medical Sciences, Mashhad, Iran)</i></p>
15.00-15.30	<p style="text-align: center;">Invited Speaker: "Theoretical Investigation on the Binding of Huperzine A and Galanthamine to Acetylcholinesterase, Based on ONIOM Method"</p> <p style="text-align: center;">Assoc. Prof. Dr. Supa Hannongbua</p> <p style="text-align: center;"><i>(Department of Chemistry, Faculty of Science, Kasetsart University, Chatuchak, Bangkok, Thailand)</i></p>
15.30-15.50	Break
15.50-16.50	Poster session II
18.00-21.00	Conference Dinner Place: Chang Sean Room (3rd Floor)
Chair: Majid Monajjemi	August 5, 2010
9.00-9.50	<p style="text-align: center;">Place: Grand Ballroom (3rd floor)</p> <p style="text-align: center;">Plenary Lecture: "Stochastic Optimization on the Quantum Conformational Space of Atomic and Molecular Microclusters"</p> <p style="text-align: center;">Prof. Dr. Albeiro Restrepo</p> <p style="text-align: center;"><i>(Grupo de Química-Física Teórica, Instituto de Química, Universidad de Antioquia, AA 1226 Medellín, Colombia)</i></p>

9.50-10.20	<p>Invited Speaker: “Cloud Computing: Recent Trends and Its Applications” Prof. Dr. Suhono Harso Supangkat <i>(Information Technology Research Division, Institut Teknologi Bandung, Indonesia)</i></p>			
10.20-10.40	Break			
10.40-11.10	<p>Invited Speaker: “A Novel Method to Identify Leucine-rich Repeats (LRRs): LRRpred” Prof. Dr. Norio Matsushima <i>(Division of Biophysics, Center for Medical Education, Sapporo Medical University, Japan)</i></p>			
11.10-11.40	<p>Invited Speaker: “Modeling Of Microsolvation Conformation Of Crown Ether-Cation Complexes by <i>Ab initio</i> Method” Prof. Dr. Harno Dwi Pranowo <i>(Austrian-Indonesian Center for Computational Chemistry (AIC), Chemistry Department, Faculty of Mathematics and Natural Sciences, Universitas Gadjah Mada, Yogyakarta, Indonesia)</i></p>			
11.40-13.00	Lunch			
13.00-13.30	<p><u>Computational Chemistry</u> Chair: Babak Khalili Hadad Grand Ballroom (3rd floor)</p>	<p><u>Computational Biology</u> Chair: Supat Jiranusornkul Chiang Dao 1 (3rd floor)</p>	<p><u>Computational Physics</u> Chair: Foroughi Abari Chiang Dao 2(3rd floor)</p>	<p><u>Computational Material Sciences</u> Chair: Alireza Ilkhani Chiang Dao 3(3rd floor)</p>
	<p>Invited Speaker: “Synthesis and Theoretical Study on Zinc(II) and Ni(II) Complexes of 5-methoxyisatin-3-(N-(4-</p>	<p>Invited Speaker: “Computational Intelligence in Biomedical Engineering Applications”</p>	<p>Invited Speaker: “Some Minimalist Dynamics” Dr.Wan Ahmad Tajuddin</p>	<p>Invited Speaker: “Computational Study of Montmorillonite-based Systems”</p>

	chlorophenyl))thiosemicarbazone ” Prof. Dr. Fatma Kandemirli (Department of Chemistry, Kocaeli University, Turkey)	Assoc. Prof. Dr. Nipon Theera-Umpon (Biomedical Engineering Center, and Department of Electrical Engineering, Faculty of Engineering, Chiang Mai University, Chiang Mai, Thailand)	Wan Abdullah (Department of Physics, Faculty of Science, and Faculty of Computer Science and Information Technology, Universiti Malaya, Malaysia)	Assoc. Prof. Hermawan K. Dipojono (Department of Engineering Physics, ITB, Indonesia)
13.30-14.00	Invited Speaker: “Design and Construction of Molecular Magnetic Materials Using Open-Shell Molecules” Prof. Dr. Naoki Yoshioka (Department of Applied Chemistry, Keio University, Japan)	Invited Speaker: “Combined Knowledge- based, Atomistic Simulation, Virtual Screening and Pharmacophoric Design Increasing Chances in Designing Hit Anti-Infectives Based on Natural Product” Assoc. Prof. Dr. Habibah A. Wahab (Division of Hits-to-Lead, Malaysia Institute of Pharmaceuticals and Nutraceuticals, Ministry of Science, Technology and Innovation, Universiti Sains Malaysia, Malaysia)	“Prediction of HEMT Transistor Noise Parameters using Computational Intelligence Method” M. Hayati (Faculty of Engineering, Razi University, Iran)	“Theoretical Study of Thermoelectric Properties of CuGaO ₂ ” P. Poopanya (Faculty of Science, Ubon Ratchathani University, Thailand)
			“Structural and Electronic Properties of Ca _{1+x} Cu _{3- x} Ti ₄ O ₁₂ by First-principles Calculation” W. Chaiyarat (Faculty of Science, Ubon Ratchathani University, Thailand)	“The Geometry and Electronic Structures of Sidewall Functionalized Carbon Nanotubes: A Theoretical Study on the Effects of Carboxylic Groups” S. Lokavee (Faculty of science, Mahidol University, Thailand)

14.00-14.30	<p>“DFT studies of behavior of B-N Bonding using by Electron Paramagnetic Resonance (EPR) at B₉N₉ nanocone”</p> <p>H. Yamola (Science and Research Branch, Islamic Azad University, Iran)</p>	<p>“The Investigation of Anti Cancer Effects of Chamomile Flower by Using <i>Ab initio</i> Method”</p> <p>M. Jorkesh (Shahriar Branch, Islamic Azad university, Iran)</p>	<p>“Simulation on Thermal Conductivity of MgO and PbTe by Molecular Dynamics Method”</p> <p>H. Wattanasarn (Faculty of Science and Technology, Sakon Nakhon Rajabhat University, Thailand)</p>	<p>“A Study of Porphine and Metal-porphine at The Gas/Water Interface Based on Molecular Dynamics Simulations”</p> <p>W. Donkrajang (Faculty of Science, Mahidol University, Thailand)</p>
	<p>“Theoretical Investigation of Molecular Structure in Octahedral Complexes of The Transition Metals”</p> <p>M. Khaleghian (Science and Research Branch, Islamic Azad University, Iran)</p>	<p>“Thermodynamic and Extended Huckel Study on The Molecule “Adriamycin P.S.F.” Anti-Cancer Drug Using QM/MM Methods”</p> <p>H. Khoshnevis (Science & Research Branch, Islamic Azad University, Iran)</p>		
14.30-14.50	Break			
14.50-15.20	<p><u>Computational Chemistry</u> Chair: Piyarat Nimmanpipug Grand Ballroom</p>	<p><u>Computational Biology</u> Chair: Vannajan Sanghiran Lee Chiang Dao 1</p>	<p><u>Computational Nanosciences</u> Chair: Mehran Hoodaj Chiang Dao 2</p>	<p><u>Computational Mathematics</u> Chair: Wan Ahmad Tajuddin Chiang Dao 3</p>
	<p>“NMR Chemical Shift Study on Nanostructure of Vinblastine by</p>	<p>Invited Speaker:</p>	<p>“First principles study of electronic structure for</p>	<p>Invited Speaker:</p>

	<p>Density Functional Theory Approach” F. Mollaamin <i>(Qom Branch, Islamic Azad University, Iran)</i></p>	<p>“Biomolecular Modeling” Assoc. Prof. Dr. Muhamad A. Martoprawiro <i>(ITB, Indonesia)</i></p>	<p>CoX₃(X= P, As, Sb)” A. Srisaikam <i>(Department of Physics, Faculty of Science, Ubon Ratchathani University, Thailand)</i></p>	<p>“Computational Problem in Reduced-Order Linear Parameter Varying Controller” Prof. Dr. Roberd Saragih <i>(Industrial and Financial Research Group, Faculty of Mathematics and Natural Science, Bandung Institute of Technology, Indonesia)</i></p>
	<p>“The Rehybridization Effect on Cyclic Compounds” S.N. Mirsattari <i>(Shahrezanext term Branch, Islamic Azad University, Iran)</i></p>		<p>“Quantum Mechanics Simulation on Excited-State Proton Transfer Reactions of 1H-Pyrrolo[3,2-h]quinoline with Methanol Clusters in the Gas Phase” R. Daengngern <i>(Department of Chemistry, Faculty of Science, Chiang Mai University, Thailand)</i></p>	
15.20-15.50	<p>“DFT study of Hydrogen Bonding on Calix[8]arene as Nanostructure Compound” M. Sayadian <i>(Islamshahr branch, Islamic Azad University, Iran)</i></p>	<p>“Structure and Function of CYP in Type 2 Diabetes Mellitus and Cataract Patients which Associated with Mitochondrial DNA Mutation” I. P. Maksum <i>(Indonesia)</i></p>	<p>“Computational Design and Study on Nano Peptide Based Stent; A Novel Strategy to an Effective Simultaneous, Angioplasty and Drug Delivery” B. K. Hadad <i>(Roudehen branch, Islamic Azad University, Iran)</i></p>	<p>“Simulation in Combined Convective and Far-infrared Radiation Drying of Fruit Leather” S. Jaturonglumlert <i>(Department of Mechanical Engineering, Faculty of Engineering, Chiang Mai University, Thailand)</i></p>

		<p>“Molecular Modeling of Cationic Porphyrins as Ligand of Radiopharmaceutical Kit”</p> <p>Ni Made Pitri Susanti (Indonesia)</p>	<p>“Computational Study of DNA Interaction with Carbon Nanotube and Approach to Drug Design”</p> <p>A. Ilkhania (Yazd Branch, Islamic Azad University, Iran)</p>	<p>“Application of the Method in the Tabu Search Optimization Clothes Pattern Laying on the Cloth”</p> <p>W. Gazali (Indonesia)</p>
15.50-16.30	Poster session III			
Chair: Nawee Kungwan	August 6, 2010			
9.00-9.30	<p>Place: Grand Ballroom (3rd floor)</p> <p>Invited Speaker: “Fixed Point Theory and Applications to Equilibrium Problems, Minimization and Variational Inequality Problems”</p> <p>Prof. Dr. Suthep Suantai (Department of Mathematics, Faculty of Science, Chiang Mai University, Chiang Mai, Thailand)</p>			
9.30-10.00	<p>Invited Speaker: “Molecular Modeling and Simulations: Applications in Biomolecular and Material Design at Chiang Mai University”</p> <p>Dr. Vannajan Sanghiran Lee (Computational Simulation and Modeling Laboratory (CSML), Department of Chemistry and Center for Innovation in Chemistry, Thailand Center of Excellence in Physics (ThEP), Faculty of Science, Chiang Mai University, Chiang Mai, Thailand)</p>			
10.00-10.30	<p>Invited Speaker: “Molecular Modeling and Study Interaction of N-(Benzoyl) penicillin derivatives to Penicillin Binding Proteins”</p> <p>Prof. Dr. Siswandono (Faculty of Pharmacy, Airlangga University, Kampus ,B Jalan Dharmawangsa Dalam Selatan, Surabaya, Indonesia)</p>			

10.30-10.50	Break			
10.50-11.20	<p style="text-align: center;"><u>Computational Chemistry</u> Chair: Anoosh Eghdami <i>Grand Ballroom</i></p>	<p style="text-align: center;"><u>Computational Biology</u> Chair: Mohammad Hassan Zadeh Khayat <i>Chiang Dao 1</i></p>	<p style="text-align: center;"><u>Computational Nanosciences</u> Chair: Reza Karbakhsh <i>Chiang Dao 2</i></p>	
	<p style="text-align: center;">“Toxicity Prediction of Some Tetrapyrrolic Macrocyclic by ECOSAR and Toxtree” A. D. Djalil <i>(Indonesia)</i></p>	<p style="text-align: center;"><i>Invited Speaker:</i> “HELFIT: A New Method of Helix Fitting” Prof. Dr. Purevjav Enkhbayar <i>(Department of Biophysics and Bioinformatics, National University of Mongolia, Mongolia)</i></p>	<p style="text-align: center;">“The Study of Burazine Nanotube Effects in Propranolol Drugs Using <i>Ab initio</i> Method” P. Farahani <i>(Science and Research branch, Islamic Azad University, Iran)</i></p>	
	<p style="text-align: center;">“Dynamics Simulation of Plasma Effect on Epoxy Resin for Dental Application” W. Sangprasert <i>(CSML, Department of Chemistry and Center for Innovation in Chemistry, Thailand Center of Excellence in Physics (ThEP), Chiang Mai University, Thailand)</i></p>		<p style="text-align: center;">“Investigation on Alcohol Nano Sensors in Combination with Carbon Nanotubes (CNTs); A Monte Carlo and <i>Ab initio</i> Simulation” M. Falahati <i>(Science and Research branch, Islamic Azad University, Iran)</i></p>	

11.20-11.50	<p>“Molecular Dynamics Simulation of Nafion Surface Modification by Ar+ Beam Bombardment” J. Yana <i>(CSML, Department of Chemistry and Center for Innovation in Chemistry, Thailand Center of Excellence in Physics (ThEP), CHE, Chiang Mai University, Thailand)</i></p>	<p>“MC Simulation and VMD Conformational Study on 1TFG And 2TGI Protein” B. K. Hadad <i>(Roudehen Branch, Islamic Azad University, Iran)</i></p>	<p>“<i>Ab initio</i> Study and NBO Analysis of Methane Absorption by Carbon Nanotube” M. Noei <i>(Mahshahr Branch, Islamic Azad University, Iran)</i></p>	
	<p>“Computational Simulation Studies on Carvedilol; To Predict Thermodynamics Properties Using DFT” K. Bakhshi <i>(Science and Research Branch, Islamic Azad University, Iran)</i></p>	<p>“Computational Study on Physico-Chemical Properties of Pure CpG Islands and Methylated Form, As A Common Feature of Human Neoplasm” B. Seify <i>(Science and research branch, Islamic Azad University, Iran)</i></p>	<p>“Modeling of 50kDa Biomarker Protein from <i>Salmonella enterica</i> Serovar Typhi” Y. S. Choong <i>(INFORMM, Malaysia)</i></p>	
11.50-13.00	Lunch			
13.00-13.30	<p><u>Computational Chemistry</u> Chair: Ahmad Ali Foroughi Abari Grand Ballroom</p>	<p><u>Computational Biology</u> Chair: Fatemeh Mollaamin Chiang Dao 1</p>	<p><u>Special Interests</u> Chair: Morrakot Khebchareon Chiang Dao 2</p>	

	<p>“Docking Study of Naproxen and Its Derivatives on Inducible Nitric Oxide Synthase” R. E. Kartasasmita <i>(Indonesia)</i></p>	<p>“QM/MM Modelling of the Reaction Mechanism of Chorismate Synthase” N. Lawan <i>(Department of Chemistry, Faculty of Science, Chiang Mai University, Thailand)</i></p>	<p>“Investigation on the impact of different median barrier shapes on a roadside environmental noise screen by Boundary Element Method” M. R. Monazzam <i>(School of Public Health, Tehran University of Medical Sciences, Tehran, Iran)</i></p>	
	<p>“Theoretical Study of the Ring-Opening Polymerization of ϵ-Caprolactone Initiated by Novel Tin(II) Alkoxides” C. Sattayanon <i>(Department of Chemistry and Center for Innovation in Chemistry, Chiang Mai University, Thailand)</i></p>	<p>“Hybrid QM/MM Simulations on the Reaction Mechanism of Chitin Hydrolysis Catalyzed by Chitinase B from <i>Serratia marcescens</i>” J. Jitonnom <i>(CSML, Department of Chemistry and Center for Innovation in Chemistry, Thailand Center of Excellence in Physics (ThEP), CHE, Chiang Mai University, Thailand)</i></p>	<p>“Simulation of Rounding Threshold and Microrotation for Punctured Radix-8 CORDIC to Reduce Hardware Complexity with Low Latency” A. Kassinook <i>(TAIST Tokyo Tech, ICTES Program, School of Information, Sirindhorn International Institute of Technology, Thammasat University, Thailand}</i></p>	

13.30-14.00	<p>“QSAR of 6-Hydroxyflavon Derivatives and Prediction of Inhibition Activity of Quercetin Derivative as α-Glucosidase Inhibitor” S. Damayanti <i>(Indonesia)</i></p>	<p>“The Effect of Dielectric Constant and Temperature Changes on The Active Site of Oxidized Azurin: An IR Study” K. Shahanipur <i>(Falavarjan Branch, Islamic Azad University, Iran)</i></p>	<p>“Monte Carlo Simulation Method for Assessment the Reinforced Concrete Structure Exposed to Chloride Environment” C. Sookoomjariyapong <i>(Department of Civil Engineering, Vongchavalitkul University, Thailand)</i></p>	
	<p>“Diterpenes from Bagore (<i>Caesalpinia crista</i> Linn.) as Antimalarial Agents: QSAR Study and Their Interaction with Plasmodium falciparum Proteases by <i>In silico</i>” M. Aswad <i>(Indonesia)</i></p>	<p>“Investigation of Thermodynamic Properties of Safranal Using DFT Method” F. Jadidi <i>(Science and Research Branch, Islamic Azad University, Iran)</i></p>	<p>“Using Artificial Neural Network for Prediction Compressive Strength of Rubber Filled Concrete” R. Masoudnia <i>(Malaysia)</i></p>	
14.00-14.30	<p>“Solvation effect on binding of postulated Succinate dehydrogenase with Ubiquinone from <i>Klebsiella pneumoniae</i> MGH78578” Sy Bing Choi Pharmaceutical Design and Simulation (PhDs) Laboratory, School of Pharmaceutical</p>	<p>“Cholesterol Effect Investigation in Point of Theta4 Angle Changing on Some Phospholipids by QM/MM Method” M. K. Takalo <i>(Science and Research Branch, Islamic Azad University, Iran)</i></p>	<p>“Numerical Investigation of Laminar Flow and Heat Transfer in A Tube with 45° Angled Ribs” P. Promvonge <i>(Department of Mechanical Engineering, Faculty of Engineering, King Mongkut's Institute of Technology</i></p>	

	Sciences, Universiti Sains Malaysia, Malaysia		<i>Ladkrabang, Thailand)</i>	
		<p>“Study in Theta4 Structural Change of DPPC and DMPC in Solvents by Various Dielectric Coefficient”</p> <p>R. Karbakhsh (<i>Science and Research Branch, Islamic Azad University, Iran</i>)</p>	<p>“Numerical Analysis of Laminar Heat Transfer in a Square Channel with Inclined Orifices”</p> <p>A. Kanarat (<i>Department of Mechanical Engineering, Faculty of Engineering, King Mongkut’s Institute of Technology Ladkrabang, Thailand</i>)</p>	
14.30-14.50	Break			
14.50-15.20	<p><u>Computational Biology I</u> Chair: <u>Narin Lawan</u> <i>Chiang Dao 1</i></p>	<p><u>Computational Biology II</u> Chair: <u>Emran K. Kartasasmita</u> <i>Chiang Dao 2</i></p>	<p><u>Special Interests</u> Chair: <u>Morrakot Khebchareon</u> <i>Chiang Dao 3</i></p>	
	<p>“Computational Alanine Scanning of ScFv Anti-P17 and HIV-1 P17 Epitope”</p> <p>P. Tue-ngeun (<i>CSML, Department of Chemistry and Center for Innovation in</i></p>	<p>“Interaction of Erythromycin A on a Single Base Substitution of 50S Ribosomal Unit”</p> <p>S.-Z. M. Zobir (<i>Malaysia</i>)</p>	<p>“Classification Students with Learning Disabilities Using Naïve Bayes Classifier and Decision Tree”</p> <p>N. Muangnak (<i>Faculty of Science and</i></p>	

	<i>Chemistry, Thailand Center of Excellence in Physics (ThEP), CHE, Chiang Mai University, Thailand)</i>		<i>Engineering, Kasetsart University, Chalermphrakiat Sakonnakhon Province Campus, Thailand)</i>	
	<p>“Investigation on Molecular Docking and Dynamics of AFB Metalloprotease and Its Propeptides Analogues”</p> <p>S. Krongdang (CSML, Department of Chemistry and Center for Innovation in Chemistry, Thailand Center of Excellence in Physics (ThEP), CHE, Chiang Mai University, Thailand)</p>	<p>“Binding Affinity of (R)- and (S)-Methadone in CYP3A4 Alleles”</p> <p>N. N. Syazana (Institute for Research in Molecular Medicine (INFORMM), Universiti Sains Malaysia, Pulau Pinang, Malaysia)</p>	<p>“Ant Colony Optimization Applied on Weekly Fleet Assignment Model”</p> <p>P. Ratprasert (Taiwan)</p>	
15.20-15.50	<p>“NQR and Solvent Effect Study of the Two Ligands of GABA Receptor”</p> <p>B. Honarparva (Science and Research Branch, Islamic Azad University, Iran)</p>	<p>“Molecular Dynamics Studies of Endoglucanase I from <i>Fusarium oxysporum</i>”</p> <p>S. Waesoho (Malaysia)</p>	<p>“Valuation of Basket Options by the Modified Implied Binomial Tree Model”</p> <p>F. J. Permana (Indonesia)</p>	
15.50-16.30	<p>Closing Ceremony/Organizing Committee Meeting</p> <p>Place: Grand Ballroom (3rd floor)</p>			