CURRICULUM VITAE

Assist. Prof. Dr. Jitrayut Jitonnom

Education

– Ph.D. Chiang Mai University.

– B.Sc. (Hons), Chiang Mai University.

Field of Specification

My research interests lie in the area of computational enzymology.
The focus enzymes are metalloenzyme and non–metalloenzyme.
These enzymes have relevance to such areas as biofuel, food,
and drug design. There is a strong emphasis on mechanistic
studies which involve a range of computational techniques, in particular
QM/MM and DFT. In addition to enzyme catalysis,
I am also interesting in computational studies of organometallic catalysis.
Jitonnom was the recipient of the Thailand Research
Fund scholarship of Thailand (MRG5680143 and TRG5880241).

Website

https://www.researchgate.net/profile/Jitrayut_Jitonnom

Awards

Year	Details	Awarded by
2545–2548	Science Achievement Scholarship of Thailand	CHE
2549	TGIST	NSTDA
2549–2553	CHE–PhD Sandwich Program	CHE
2556–2558	Research Grant for New Scholar (MRG)	TRF
2557	Outstanding Abstract Award	Protein Society of Thailand
2558–2560	TRF Grant for New Researcher (TRG)	TRF
2560	Certificate of Recognition in *Journal of Physical Chemistry B*	*ACS, USA*
2560	Certificate of Invited Lecture	DIPC, Spain
2560	Certificate of Poster Presentation	DIPC, Spain
2560	Certificate of Reviewing in *Journal of Organometallic Chemistry*	Elsevier, Netherland

TRF = Thailand Research Fund

NSTDA = National Science and Technology Development Agency

CHE = The Commission on Higher Education

TGIST = Thailand Graduate Institute of Science and Technology

DIPC = Donostia International Physics Center, Spain (http://dipc.ehu.es/)

ACS = American Chemical Society (https://www.acs.org/content/acs/en.html)

ผลงานวิจัย (Research)

2018

1. **Jitonnom J.**, Hannongbua S. Theoretical study of the arabinan hydrolysis by an inverting GH43 arabinanase, Mol. Simul. 2018, 44(8), 631–637.
2. **Jitonnom J.** Data characterizing the energetics of enzyme–catalyzed hydrolysis and transglycosylation reactions by DFT cluster model calculations. Data Brief, 2018, 17, 788–795. (SCOPUS/ISI)
3. **Jitonnom J.**, Ketudat–Cairns JR., Hannongbua S. QM/MM modeling of the hydrolysis and transfructosylation reactions of fructosyltransferase from Aspergillus japonicas, an enzyme that produces prebiotic fructooligosaccharide. J. Mol. Graph. Model. 2018, 79, 175–184. (SCOPUS/ISI)

2017

1. **Jitonnom J.**, Meelua W. Cationic ring–opening polymerization of cyclic carbonates and lactones by group 4 metallocenes: A theoretical study on mechanism and ring–strain effects. J. Theor. Comp. Chem., 2017, 16(1), 1750003.
2. **Jitonnom J.**, Meelua W. Effect of ligand structure in the trimethylene carbonate polymerization by cationic zirconocene catalysts: A “naked model” DFT study. J.Organometal. Chem., 2017, 841, 48–56.
3. **Jitrayut Jitonnom,** Jon I. Mujika, Marc W. van der Kamp, Adrian J. Mulholland. Quantum Mechanics/Molecular Mechanics Simulations Identify the Ring–Opening Mechanism of Creatininase. J. Phys. Chem. B, 2017, 56, 6377–6388.

2016

1. **Jitonnom J.**, Molloy R., Punyodom W., Meelua W. Theoretical studies on aluminumtrialkoxide–initiated lactone ring–opening polymerizations: Roles of alkoxide substituentand monomer ring structure. Comput. Theor. Chem. 2016, 1097, 25–32. (SCOPUS/ISI)

2. Sangwijit K., **Jitonnom J.**, Pitakrattananukool S., Yu L.D., Anuntalabhochai S.Low–energy plasma immersion ion implantation modification of bacteria to enhance hydrolysis of biomass materials. Surf. Coat. Technol. 2016, 306A, 336–340. (SCOPUS/ISI)
3. Cheenpracha S., **Jitonnom J.**, Komek M., Ritthiwigrom T., Laphookhieo S., Acetylcholinesterase inhibitory activity and molecular docking study of steroidal alkaloids from Holarrhena pubescens barks. Steroids 2016, 108, 92–98. (SCOPUS/ISI)
4. **Jitonnom J.**, Sontag C. Catalytic oxidation of glucose with hydrogen peroxide and colloidal gold as pseudo–homogenous catalyst: a combined experimental and theoretical investigation, Chiang Mai J. Sci. 2016, 43(4), 825–833. (SCOPUS/ISI)

2015

1. **Jitonnom J.**, Sattayanon C., Kungwan N, Hannongbua S., A DFT study of theunusual substrate–assisted mechanism of Serratia marcescens chitinase B reveals the role of solvent and mutational effect on catalysis. J. Mol. Graph.Model. 2015, 56, 53–59.(SCOPUS/ISI)

2014

1. **Jitonnom J.**, Meelua W. The effect of silicon–bridge and p–ligands on the electronic structures and related properties of dimethyl zirconocene polymerization catalysts: A comparative theoretical investigation, Chiang Mai J. Sci. 2014, 41(5.2): 1220–1229.(SCOPUS/ISI)
2. Sattayanon C., Sontising W., **Jitonnom J.**, Meepowpan P., Punyodom W., Kungwan N. Theoretical study on the mechanism and kinetics of ring–opening polymerization of cyclic esters initiated by tin(II) n–butoxide. Comput. Theor. Chem. 2014, 1044, 29–35.(SCOPUS/ISI)
3. **Jitonnom J.**, Limb M.A., Mulholland A.J. QM/MM free–energy simulations of reaction in Serratia marcescens chitinase B reveal the protonation state of Asp142 and the critical role of Tyr214. J. Phys. Chem. B. 2014, 118, 4771–83. (SCOPUS/ISI)

2012

1. **Jitonnom J.**, Sontag C. Comparative study on activation mechanism of carboxypeptidase A1, A2 and B: First insights from steered molecular dynamics simulations. J. Mol. Graph.Model. 2012, 38C, 298–303. (SCOPUS/ISI)
2. **Jitonnom J.**, Mulholland A. Insights into conformational changes of procarboxypeptidase A and B from simulations: a plausible explanation for different intrinsic activity. Theor. Chem. Account., 2012, 131, 1–13. (SCOPUS/ISI)
3. **Jitonnom J.**, Lomthaisong K., Lee V.S. Computational Design of Peptide Inhibitor Based on Modifications of Proregion from Plutella xylostella Midgut Trypsin. Chem. Biol. Drug Des. 2012, 79, 583–93. (SCOPUS/ISI)

2011

1. **Jitonnom J.**, Lee V.S., Nimmanpipug P., Rowlands H.A., Mulholland A.J. Quantum mechanics/molecular mechanics modeling of substrate–assisted catalysis in family 18 chitinases: conformational changes and the role of Asp142 in catalysis in ChiB. Biochemistry. 2011, 50, 4697–711. (SCOPUS/ISI)
2. **Jitonnom J.**, Mulholland A.J., Nimmanpipug P., Lee V.S. Hybrid QM/MM study on the deglycosylation step of chitin hydrolysis catalyzed by chitinase B from Serratia marcescens, Maejo Int. J. Sci. Technol. 2011, 5(1), 47–57. (SCOPUS/ISI)
3. Yakhantip T., Kungwan N., **Jitonnom J.**, Anuragudom P., Jungsuttiwong S., Hannongbua S. Theoretical investigation on the electronic and optical properties of poly(fluorenevinylene) derivatives as light–emitting materials Int. J. Photoenergy, vol.2011, Article ID 570103, 9 pages, 2011. (SCOPUS/ISI)

2010

1. Lee V.S., Kodchakorn K., **Jitonnom J.**, Nimmanpipug P., Kongtawelert P., Premanode B. Influence of metal cofactors and water on the catalytic mechanism of creatininasecreatinine in aqueous solution from molecular dynamics simulation and quantum study, J. Comput. Aided Mol. Des. 2010, 24, 879–886. (SCOPUS/ISI)
2. Lee V. S., Tuengeun P., Nangola S., Kitidee K., **Jitonnom J.**, Nimmanpipug P., Jiranusornkul S., Tayapiwatana C., Pairwise decomposition of residue interaction energies of single chain Fv with HIV–1 p17 epitope variants, Mol. Immuno. 2010, 47, 982–990. (SCOPUS/ISI)

2007

1. Nimmanpipug P., **Jitonnom J.**, Ngaojampa C., Hannongbua S, Lee V.S., A computational H5N1 neuraminidase model and its binding to commercial drugs. Mol. Simul. 2007, 33, 487–493. (SCOPUS/ISI)
2. Nimmanpipug P., Junkaew A., **Jitonnom J.**, Lee V.S. Polymerizability of lactones calculated by molecular mechanics, semiempirical and density functional theory methods. Chiang Mai J. Sci. 2007, 34, 1–9. (SCOPUS/ISI)