

Yossa Dwi HARTONO

PERSONAL DATA

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WEBPAGE yossadh.github.io

WORK

2018– Research Fellow, **National University of Singapore (NUS)**
Synthetic Biology for Clinical and Technological Innovation (SynCTI),
Department of Biochemistry, Yong Loo Lin School of Medicine
&
Research Fellow (Collaborator), **Bioinformatics Institute (BII)**
Agency for Science, Technology and Research (A*STAR), Singapore
Project: Structure-guided enzyme design and engineering
Supervisors: YEW Wen Shan (NUS), FAN Hao (BII)

EDUCATION

2012–2017 PhD in COMPUTATIONAL BIOPHYSICS, **Karolinska Institutet, Sweden**
Jointly awarded by **Nanyang Technological University, Singapore**
Thesis: [Understanding structural features of biomolecular interactions: from classical simulations to *ab initio* calculations](#)
Supervisors: Alessandra VILLA, Lennart NILSSON, Konstantin PERVUSHIN

2008–2012 BSc in CHEMISTRY AND BIOLOGICAL CHEMISTRY
with concentration in MEDICINAL CHEMISTRY
First Class Honours, GPA: 4.64/5.00
Nanyang Technological University, Singapore
Thesis: Polymeric surfactant-based drug delivery technology for poorly water soluble drugs
(done as internship in Abbott Laboratories, now AbbVie)
Advisor: Xueming LIU

RESEARCH SKILLS AND EXPERIENCE

Undergraduate research (2009–2011)

- Docking with AutoDock
- Molecular dynamics simulation with AMBER
- Binding energy approximation with MM-PBSA

Undergraduate honours thesis, Abbott Laboratories (2012)

- HPLC
- Spray drying
- Dynamic light scattering
- Differential scanning calorimetry
- Dissolution testing

PhD (2012–2014)

- Protein overexpression in *E. coli*
- Immobilised metal affinity chromatography
- Size-exclusion chromatography
- Ion-exchange chromatography
- NMR spectroscopy

- Screening for X-ray crystallography.

PhD (2014–2017)

- Molecular dynamics simulation with CHARMM
- λ -dynamics as a tool to study protonation and tautomerisation in nucleic acids
- Free energy calculations
- Umbrella sampling
- QM/MM with Q-Chem/CHARMM

Research fellowship (2018–)

- Scripting with Bash and Python
- Homology modelling with MODELLER
- Molecular docking with DOCK 3.6, Schrödinger Glide, GOLD
- Molecular dynamics simulation with GROMACS

TEACHING

- Supervising two high school students for small project in our group (2-week project, Nov/Dec 2016, in Karolinska Institutet): Introducing structural biology and molecular simulation.
- Teaching assistant for Structural Biology, 1-week Biomedicine undergraduate course in Karolinska Institutet, in 2015, 2016, and 2017: Teaching 3D molecular visualisation with RasMol and marking assignments.
- Supervising an undergraduate for one-semester research NMR project in Nanyang Technological University, in 2013: Mentoring, overseeing project and final report.
- Teaching assistant for Molecular Evolution course, Biological Sciences undergraduate course over 1 semester in Nanyang Technological University, in 2013: Marking assignments.
- Teaching assistant for Biochemistry I, Principle of Genetics, Principles and Methods of Biophysics, Biological Sciences undergraduate courses over 1 semester in Nanyang Technological University, in 2012-2013: Supervising laboratory practicals and marking reports.

CONFERENCES AND PRESENTATIONS

- EMBO workshop "RNA structure meets function"
12-15 Jun 2016 | Stockholm Archipelago, Sweden
Poster: Tautomerisation and protonation equilibria of nucleic acids
- The 13th Greta Pifat-Mrzljak International School of Biophysics
1-10 Sep 2016 | Split, Croatia
Poster and short talk: Protonation of cytidine and tautomerisation of pseudoisocytidine: λ -dynamics study
- International Society of Quantum Biology and Pharmacology President's meeting
19-22 Jun 2016 | Bergen, Norway
Poster: Keto-enol tautomerisation of modified uridine in ribosome decoding centre
- Department of Biosciences and Nutrition, Internal Seminar
14 Apr 2016 | Stockholm, Sweden
Short talk: Base-flipping in triplex nucleic acids
- Uppsala-Stockholm Workshop on Biomolecular Simulation
13 Dec 2016 | Uppsala, Sweden
Short talk: Tautomerisation of pseudoisocytidine: λ -dynamics study
- Uppsala-Stockholm Workshop on Biomolecular Simulation
19 Oct 2015 | Stockholm, Sweden
Short talk: Investigating protonation and tautomerisation with λ -dynamics

- Annual Meeting of the Swedish Chemical Society, Theoretical Chemistry Section
25-27 Aug 2015 | Kalmar, Sweden
Poster: Base-flipping of cytidine in triplex nucleic acids
- EMBO workshop "Advances in protein-protein interaction analysis and modulation"
9-12 Sept 2014 | Hyères, France
Poster: Dynamics of giant viral homologues of human eRF1

AWARDS AND SCHOLARSHIPS

2012-2016	NTU Research Scholarship
2008-2012	ASEAN Undergraduate Scholarship
2006-2007	ASEAN Scholarship
2006	Singapore Chemistry Olympiad, Bronze Award
2004-2005	Singapore Ministry of Education School-based Scholarship

LANGUAGES

INDONESIAN/MALAY	Native
ENGLISH	Fluent
SWEDISH	Elementary

OTHER ACTIVITIES

- Apr 2019: Competed in Public Service Swimming Meet 2019.
- Nov 2018: Competed in Singapore Masters Short Course Swimming Championships 2018. 3rd place in age group 30-34 category for 25m breaststroke, 25m backstroke and 50m breaststroke.
- 2018-: Member of NUS Staff Swim Team (Vice-Captain, 2020-)
- 2016-2017: Blogger at Karolinska Institutet [Research and Career Blog](#). Writing about science for the laypeople, philosophy of science, and science communication.
- 2015-2017: Member of Master Swim group in Stockholm Student Sport Association (*Stockholms Studenter Idrotts Föreningen*).
- 2011, 2012: Volunteer in Anti-doping section for FINA/Arena Swimming World Cup.
- 2011-2013: Member of NTU Lifeguard Corps (Secretary, Academic Year 2012-2013). Certified pool lifeguard and competed in Singapore national and varsity lifesaving competitions.
- 2008-2009: Member of NTU Mentoring. Giving voluntary tuition in Science and Mathematics to Secondary School students (equivalent to grades 9 and 10).
- 2008-2011: Live-in tutor in Anglo-Chinese School (Independent) Boarding School. Duties include giving tuition, supervising students' study time, looking after students' well-being, attending residential staff meeting, and lifeguard service at swimming pool facility.

Published

- Hartono, Y. D.[†]; Xu, Y.[†]; Karshikoff, A.; Nilsson, L.; Villa, A. Modeling pK shift in DNA triplexes containing locked nucleic acids *J. Chem. Info. Model.* **2018**, DOI: 10.1021/acs.jcim.7b00741 [†]Equal contribution
- Hartono, Y. D.; Ito, M.; Villa, A.; Nilsson, L. A computational study of uracil tautomeric forms in the ribosome: the case of uracil and 5-oxyacetic acid uracil in the first anticodon position of tRNA. *J. Phys. Chem. B* **2017**, 5, 2165-2177, DOI: 10.1021/acs.jpcc.7b10878
- Hartono, Y. D.; Y. Pabon, V.; Uyar, A.; Wengel, J.; Lundin, K.E.; Zain, R.; Smith, C.I.E.; Nilsson, L.; Villa, A. Role of pseudocytidine tautomerization in triplex forming oligonucleotides: in silico and in vitro studies. *ACS Omega* **2017**, 5, 2165-2177, DOI: 10.1021/acsomega.7b00347.
- Hartono, Y. D.; Yip, Y. M.; Zhang, D. Folding dynamics and adsorption of MPER of HIV-1 gp41 in the presence of DPC micelle. *Proteins: Structure, Function, and Bioinformatics* **2013**, 81, 933-944, DOI:10.1002/prot.24256.
- Hartono, Y. D.; Lazim, R.; Yip, Y. M.; Zhang, D. Computational study of bindings of HK20 Fab and D5 Fab to HIV-1 gp41 *Bioorgan. Med. Chem. Lett.* **2012**, 2, 4, 1695-1700.
- Hartono, Y. D.; Lee, A. N.; Lee-Huang, S.; Zhang, D. Computational study of bindings of HL9, a nonapeptide fragment of human lysozyme, to HIV-1 fusion protein gp41. *Bioorgan. Med. Chem. Lett.* **2011**, 21, 1607-1611.
- Lee, A. N.; Hartono, Y. D.; Sun, T.; Leow, M. L.; Liu, X.-W.; Huang, X.; Zhang, D. Molecular dynamics studies of human receptor molecule in hemagglutinin of 1918 and 2009 H1N1 influenza viruses. *J. Mol. Model.* **2010**, 17, 7, 1635-1641.

Other

- *PhD thesis chapter:* Hartono, Y. D.; Pervushin, K. *Megavirales* homologues of translation termination factor eRF1: protein purification and homology modelling. **2017**
- *Acknowledgment:* Irwan, A. W., Berania; J. E.; Liu, X. A comparative study on the effects of amphiphilic and hydrophilic polymers on the release profiles of a poorly water-soluble drug. *Pharma. Dev. Technol.*, **2016**, 21, 231-238.