Yossa Dwi Hartono

Personal Data

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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 equlibria 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.
- 2018–2021: Member of NUS Staff Swim Team
- 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.

Manuscripts and Publications

Published

- Hartono, Y. D.†; Xu, Y.†; Karshikoff, A.; Nilsson, L.; Villa, A. Modeling p*K* 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 anti-codon position of tRNA. *J. Phys. Chem. B* **2017**, *5*, 2165-2177, DOI: 10.1021/acs.jpcb.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 pseudoisocytidine 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.

References

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Dr Zhang Dawei
School of Physics and Engineering
Henan University of Science and Technology
(Formerly:
Assistant Professor
School of Physical and Mathematical Sciences
Nanyang Technological University, Singapore)
Relation: Undergraduate research supervisor
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