

# Yossa Dwi HARTONO

## PERSONAL DATA

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WEBPAGE [yossadh.github.io](http://yossadh.github.io)

## WORK

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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

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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

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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
- $\lambda$ -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
- Docking with DOCK 3.6, Schrödinger Glide, GOLD

## TEACHING

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- 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

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- 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:  $\lambda$ -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:  $\lambda$ -dynamics study
- Uppsala-Stockholm Workshop on Biomolecular Simulation  
19 Oct 2015 | Stockholm, Sweden  
Short talk: Investigating protonation and tautomerisation with  $\lambda$ -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

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- 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

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|------------------|------------|
| INDONESIAN/MALAY | Native     |
| ENGLISH          | Fluent     |
| SWEDISH          | Elementary |

## OTHER ACTIVITIES

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- 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
- 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

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### 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.

### 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
- 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.

\*Equal contribution