SITI AZMA JUSOH

PhD Computational Biology

Senior Lecturer/Researcher

CONTACT

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Bandar Puncak Alam, Selangor

Linkedin: www.Linkedin.com/in/sitiazmajusoh/

COMPUTING SKILLS

- Molecular Dynamics Simulations: GROMACS, Amber
- Virtual Screening: Schrodinger GLIDE, Autodock Vina
- Protein Structure Prediction
- Protein Sequence Analysis
- Web Development: Joomla!
- Data Analytics: R programming, Python
- 3D Printing: FDM, SLA, Ultimaker, Creality
- Computer-Aided Design: Autodesk Fusion 360, TinkerCAD, Autodesk Meshmixer

CURRENT POSITIONS

Head of Department
Department of Life Sciences

Senior Lecturer/Researcher
Faculty of Pharmacy
Universiti Teknologi MARA (UiTM), Malaysia.

Associate Research Fellow
Institute of Pathology, Laboratory and Forensic Medicine (I-PPerForM), UiTM

Fellow for Collaborative Group-Makerspace
Centre for Innovative Delivery & Learning Development (CIDL), UiTM

Coordinator (2018-Present)
MAKERLAB UiTM
www.makerlabuitm.my

EDUCATION

2014-2016 Postdoctoral Scholar
University of California San Diego (UCSD), USA

2006-2010 PhD in Computational Biology
Saarland University-Germany (2006-2010)

2000-2003 MSc Genetics
Universiti Kebangsaan Malaysia

1997-2000 BSc (Hons) Biotechnology with Management
Universiti Kebangsaan Malaysia

WORK/INDUSTRY EXPERIENCE

2017- 2018 - Special Officer to the Group CEO
PKT Logistics Group Sdn Bhd,
Shah Alam Selangor.

2003-2005 Research Officer
UKM Medical Molecular Biology Institute (UMBI),
Hospital UKM, Cheras, Kuala Lumpur

Research Profile

RESEARCH AREAS

- Computer-Aided Drug Design: High-throughput Virtual Screening, Ensemble-based Docking, Protein Modeling, Structure-based Drug Design
- Molecular Dynamics (MD) Simulations: Atomistic and Coarse-Grained MD, Membrane Proteins, Small molecule-Protein Interactions.

RESEARCH PROJECTS

- Interactions of small-molecule compounds with nuclear receptors.
- SARS-CoV-2 Inhibitors/Drugs
- Modeling and Dynamics of Envelope Glycoproteins of Flaviviridae Viruses: Dengue and Hepatitis C viruses.
- Structural Dynamics of Membrane Proteins in Lipid Bilayer.

Other INTERESTS

- 3D Modeling & 3D Printing Applications
- Makerspace/Fablab in Education
- Industrial Revolution 4.0 Technologies (Additive Manufacturing, Internet of Things, Drone, VR/AR/MR).
- High Performance Computing (HPC), GPU Custers for HPC & Could Computing
- Data Analytics

JOURNAL REVIEWER

- Malaysian Journal of Biochemistry & Molecular Biology
- 2021 - Present - Fab16 Conference (Fab16.org) Proceeding.
- 2020 - Present - Journal of Molecular Docking (JMD)
- 2014 - Present - Journal of Chemical Biology and Drug Design (CBDD), Wiley - Impact Factor 2.396
- 2016 - Journal of Molecular Liquids, Elsevier- Impact Factor 3.187
- 2013 Journal of the American Chemical Society (JACS), ACS Publications - Impact Factor 13.858 (2016)

SOCIETY MEMBERSHIP

- 2012-Present | Member, Malaysian Biochemistry and Molecular Biology Society (MBMMS)
- 2020 | Member, Biophysical Society
- 2018 | Committee Member, Malaysia Bioinformatics Network (MyBioinfoNet)
- 2014-2016 Member, American Chemistry Society (ACS)

FUNDING

PRINCIPAL INVESTIGATOR (Total of RM559,000)

- **2022-2024 | RM30,000** - Grant: Dana UiTM Cawangan Selangor (DUCS) - Pembudayaan Penyelidikan. Project: SARS-CoV-2 (COVID-19) Rational Drug Design Targeting the Main Protease Potential Allosteric Binding Sites.
- **2020 - 2021 | RM 100,000** - Grant: Structured Entrepreneurial Incubator Program (SEIP) by Universiti Malaysia Kelantan | Project: Ico-Works by MAKERLAB UiTM, a startup incubator for digital & creative industries.
- **2019 | RM 80,000** - Grant: Makers@University by KPT-MITI | Project: IR4.0 Training & Program in makerspace of Higher Education (Completed)
- **2018 | RM 50,000** - Tabung Amanah UiTM Cawangan Selangor (UCS) | The funding for the development of MAKERLAB UiTM in Kampus Puncak Alam. More info: www.makerlabuitm.my (Completed)
- **2017-2019 | RM 40,000** - Bestari Grant, UiTM | Research Project: Single Nucleotide Polymorphism (SNP) Effects of the OTCase Structure & Functions - A study using Molecular Dynamics Simulations. (Completed).
- **2012-2014 | RM 30,000** - Grant: Cluster Computing Grant by UiTM | Project: Structure & Dynamics of Envelope Glycoproteins Form Flaviviridae Viruses. (Completed).
- **2012-2015 | RM 142,000** - Exploratory Research Grant Scheme (ERGS) | Research Project: Molecular Modeling And Docking Studies of P-glycoprotein. (Completed)
- **2011-2013 | RM 117,000** Fundamental Research Grant Scheme (FRGS) | Research Project: Modeling And Dynamics of The Transient Receptor Potential (TRP) Channels. (Completed)

Co-Investigator (Total of RM 484,000)

- **2020-2021 | RM 25,000** - Funding UiTM | Research Project: MORPHOLOGICAL AND DIMENSIONAL ANALYSIS OF 3D METAL PRINTING BY FUSED DEPOSITION MODELING (FDM). (On-going)
- **2020-2021 | RM 25,000** - Funding UiTM | Research Project: 3D PRINTING AND SINTERING BEHAVIOUR OF STAINLESS STEEL 316L METAL FILAMENT. (On-going)
- **2019-2021 | RM128,000** - Fundamental Research Grant Scheme (FRGS) | Research Project: Modelling of Inflammatory Biomarkers DNA Methylation Profile in the Progression of Premature Atherosclerosis in Rats. (On-going)
- **2018-2020 | FRGS RM98,000** - Fundamental Research Grant Scheme (FRGS) | Project: Deciphering the Inhibitory Mechanism of Bile Pigments on Tobacco Carcinogenesis. (On-going)
- **2014-2017 | RM128,000** - Exploratory Research Grant Scheme (ERGS) | Research Project: Synthesis Of Supramolecule By Self-assembly Of Multi Dimeric Zn2+-cyclen Complexes, Organic Anions And Metal Ions In Aqueous. (Completed)
- **2014-2017 | RM80,000** - RAGS UiTM | Project: Unravelling Insulin Receptor And Its Regulators In Activating The Insulin Signaling Pathway In Induced-insulin Resistance Model Treated With Stevioside. (Completed)

PUBLICATIONS

1. 2022 Razman, Aimi Zafira, et al. "Undertreatment and Underachievement of LDL-C Target among Individuals with High and Very High Cardiovascular Risk in the Malaysian Community." *Healthcare*. Vol. 10. No. 12. MDPI, 2022. (Q1)
2. 2021 Jusoh, Siti Azma, & Nik Muhammad, Nik Maheran. (2021). A model makerspace for the digital and creative start-up entrepreneurs. Proceedings of the Fab 16 Research Papers Stream, 131–140. https://doi.org/10.5281/zenodo.5169838
3. 2018 Hio K.T., Jusoh S.A. and Shirley W.I. Siu, Chaos-embedded particle swarm optimization approach for protein-ligand docking and virtual screening. Journal of Cheminformatics (Q1: IF 5.514)
4. 2018 Ali EZ., et al. 2018 Mutation Study of Malaysian Patients with Ornithine Transcarbamylase Deficiency: Clinical, Molecular, and Bioinformatics Analyses of Two Novel Missense Mutations of the OTC Gene. BioMed Research International. (Q2: IF 3.41)
5. 2017 Han C., Marcus C. K. N., Jusoh S. A., Hio K. T., Shirley WI Siu., 2017. TMDIM: an improved algorithm for the structure prediction of transmembrane domains of bitopic dimers. Journal of Computer-Aided Molecular Design pp 1-11. (Q1; IF 3.028)
6. 2017 Akbar, R., Jusoh, S.A., Amaro, R.E. and Helms, V., 2017. ENRI: A tool for selecting structure-based virtual screening target conformations. Chemical Biology & Drug Design. (Q2; IF 2.396)
7. 2016 Swift, R.V., Jusoh, S.A., Offutt, T.L., Li, E.S. and Amaro, R.E., 2016. Knowledge-Based Methods to Train and Optimize Virtual Screening Ensembles. Journal of Chemical Information and Modeling, 56(5), pp.830-842. (Q1; IF 3.760)
8. 2016 Ismail NA, Jusoh SA, 2016. Molecular Docking and Molecular Dynamics Simulation Studies to Predict Flavonoid Binding on the Surface of DENV2 E Protein. Interdisciplinary Sciences: Computational Life Sciences. 11:1-3. (Q3; IF 1.4)
9. 2013 Beck A, Speicher T, Stoerger C, Sell T, Dettmer V, Jusoh SA, Abdulmughni A, Cavalié A, Philipp SE, Zhu MX, Helms V, 2013. Conserved gating elements in TRPC4 and TRPC5 channels. Journal of Biological Chemistry, 288(27):19471-83. (Q1; IF 4.125)
10. 2013 Akbar R, Jusoh SA. 2013. Stability, orientation and position preference of the stem region (residues 689-703) in Hepatitis C Virus (HCV) envelope glycoprotein E2: a molecular dynamics study. F1000Research, pp 2. (Q1)
11. 2013 Shaharom RR, Nayan MN, Radzi MM, Akbar R, Jusoh SA, 2013. Molecular docking study of a tocotrienol and P-glycoprotein. In Computers & Informatics (ISCI), IEEE Symposium, pp. 147-151.
12. 2013 Sarbini S, Nayan MN, Chik WW, Radzi MM, Akbar R, Jusoh SA, 2013. Molecular docking studies of a quassinoid and P-glycoprotein. In Computers & Informatics (ISCI), 2013 IEEE Symposium, pp. 138-142.
13. 2012 Chik, W.D.W., Mohamed, R., Majeed, A.B.A. and Jusoh, S.A., 2012, September. Sequence analysis and homology modeling of TRPV5 and TRPV6 channels. In Business, Engineering and Industrial Applications (ISBEIA), Bandung, Indonesia, IEEE Symposium, pp. 342-346
14. 2012 Homology Modeling of the DNA Binding and Dimerization Partner Domains of E2F1 Transcription Factor Protein in Homo sapiens. IEEE Symposium on Business, Engineering & Industrial Applications (ISBEIA 2012), Bandung, Indonesia. Sep 23-26.
15. 2011 Jusoh SA, Helms V. Helical integrity and microsolvation of transmembrane domains from Flaviviridae envelope glycoproteins. Biochimica et Biophysica Acta (BBA)-Biomembranes. 2011 Apr 30;1808(4):1040-9. (Q1: 3.747)
16. 2010 Jusoh SA, Welsch C, Siu SW, Böckmann RA, Helms V. Contribution of charged and polar residues for the formation of the E1–E2 heterodimer from Hepatitis C Virus. Journal of Molecular Modeling. 2010, 1;16(10):1625-37.
17. 2005 Abdullah, R., Zainal, A., Yew Heng, W., Chui Li, L., Chee Beng, Y., Mei Phing, L., Abdullah Sirajuddin, S., Soo Ping, W.Y., Lourdes Joseph, J. and Azma Jusoh, S., 2005. Immature embryo: A useful tool for oil palm (Elaeis guineensis Jacq.) genetic transformation studies. Electronic Journal of Biotechnology, 8(1), pp.24-34.

ORAL/POSTER PRESENTER

2020-2023

1. Young Investigator Award - 6th Asian Pacific Society of Atherosclerosis and Vascular Disease Congress 2023, Kuala Lumpur. **E498A AND R499G VARIANTS OF PCSK9 ENHANCED PCSK9-LDLR BINDING - INSIGHT FROM MOLECULAR DYNAMICS SIMULATIONS**. Oral Presentation by Nur Alya Amira Azhar (MSc).
2. 47th Annual Conference of The Malaysian Society for Biochemistry and Molecular Biology, Kuala Lumpur. **MOLECULAR INTERACTIONS OF KRATOM ALKALOIDS : MITRAGYNINE , 7-HYDROXYMITRAGYNINE AND MITRAGYNINE PSEUDOINDOXYL WITH DPPC LIPID BILAYERS**. Poster Presentation by Nur Syahirunelisa Mohd Zubri (MSc).
3. Best Poster Award - 7th Annual Conference of The Malaysian Society for Biochemistry and Molecular Biology, Kuala Lumpur. **Binding of Indinavir and Nirmatrelvir to the Dimer Pocket Interface of the SARS-CoV-2 Main Protease.** Poster Presentation by Nur Aqasyah Amran (MSc)
4. 47th Annual Conference of The Malaysian Society for Biochemistry and Molecular Biology, Kuala Lumpur. **MOLECULAR DOCKING AND MOLECULAR DYNAMIC SIMULATIONS TO EXPLORE THE POTENTIAL OF PHYTOCOMPOUNDS FROM HOPEA AS INHIBITORS TARGETING THE SARS-COV-2 MAIN PROTEASE**. Oral Presentation by Nur Hannani Ahmad Rozani (MSc)
5. Best Poster Award - 7th Annual Conference of The Malaysian Society for Biochemistry and Molecular Biology, Kuala Lumpur. **STRUCTURAL EFFECT OF PCSK9 MUTATIONS - A STUDY USING MOLECULAR DYNAMICS SIMULATIONS**. Poster Presentation by Nur Alya Amirah Azhar (MSc)
6. **3D Printing as the Core Module in the Higher Education Makerspace.** Symposium: Reimagining the Futures of 3D Printing in Society, organized by Karlsruhe Institute of Technology (KIT), Germany. (Poster Presenter). Symposium Link: https://www.itas.kit.edu/english/events_2021_re-imagining_futures_of_3d_printing.php
7. **Potential Novel Drug Binding Pockets of SARS-CoV-2 Main Protease.** MSBMB-Taylor's Virtual Focused Meeting: Viral Infections, Nov 19-2020. (Poster/Oral Presenter) Link: https://msbmb2010.wixsite.com/msbmbtu-vfm
8. 64th **Annual Meeting of the Biophysical Society**, February 15 – 19, 2020, San Diego, California. (Poster Presenter)

ORAL/POSTER PRESENTER

2019-2010

1. **4th International Conference on Computation for Science and technology (ICCST) 2016**, Langkawi 3-4 Nov, **2016.** (Oral Presenter)
2. **251st American Chemistry Society (ACS) National Meeting** - Computers in Chemistry, San Diego - USA. **March 13-17, 2016**. Title: Molecular dynamics-generated ensemble structures improve virtual screening performance. Jusoh, S.A., Swift, R.V., and Amaro, R.E. (Oral Presenter)
3. **251st American Chemistry Society (ACS) National Meeting** - Computers in Chemistry, San Diego - USA. **March 13-17, 2016.** ENRI: Enriching Virtual Screening Through Machine Learning. Akbar, R., Jusoh, S.A., Amaro, R.E. and Helms, V. (Poster)
4. **3rd Annual Postdoctoral Research Symposium**-UC San Diego-USA, **Aug 14- 2015**. Enhance Performance of Virtual Screening using MD Ensembles. Jusoh, S.A., Swift, R.V., and Amaro, R.E. (Poster)
5. **LRGS Dengue Colloquium and Workshop**, 11-14th June **2013**. Interaction of TMD of E protein of Dengue Virus with Lipids: A Molecular Dynamics Study. University of Malaya, Kuala Lumpur. (Invited Speaker)
6. **Conference on Membrane Protein Structure and Function**, Suzhou, March 13-17, **2013.** Contribution of Soluble Region to Transmembrane Helix: Structural Stability and Heterodimerization of Hepatitis C Virus Envelope Glycoprotein E1-E2. (Poster)
7. Structural Bioinformatics of Integral Membrane Protein. **IEEE Symposium on Computer & Informatics** (ISCI) **2012**, Penang. (Oral Presenter).
8. MD simulations of Bitopic Helices from Envelope Glycoprotein of Flaviviridae Viruses. **Annual Symposium on Recent advances in Membrane Biochemistry**, Cambridge-UK, Jan 5-6 **2011.** (Poster).
9. **Workshop on Computer Simulation and Theory of Macromolecules**, Hünfeld-Germany, 15-16th Mac **2010**. Molecular Dynamic Simulation as an Alternative Approach to Study the Behavior of Charged and Polar Residues in the Transmembrane Domains of Envelope Glycoprotein of Flaviviridae Virus Family. (Oral Presenter)

SEMINAR/WORKSHOP ORGANIZER

ORGANIZER

- **2023 |** Hands-on Workshop on Bioinformatics for Life Sciences & Drug Design, Faculty of Pharmacy, UiTM Puncak Alam, Mar 13-17.
- **2022 |** Hands-on Workshop on Bioinformatics for Life Sciences & Drug Design, UiTM Shah Alam, Mar 14-18.
- **2018 |** Workshop on Basic Molecular Docking - Bioinformatics Lab, Faculty of Pharmacy, UiTM, April 6.
- **2017 |** Co-organizer for the 10th International Conference on Computational Biophysics (ICCP10), MACAU, Jan 16-20.
- **2016 |** Workshop on Docking & Protein Modeling - 7th International Conference on Computational System-Biology and Bioinformatics (CSBio-2016), MACAU, Dec 19-22.
- **2013 |** Workshop on the Protein Structure Prediction for Diagnostics Application, Institute for Medical Research (IMR), Kuala Lumpur, May 28-30.
- **2013 |** Workshop on the Protein Modeling & Docking, Bioinformatics Lab, Faculty of Pharmacy, UiTM Puncak Alam, Dec 2-6.
- **2013 |** Professorial Lectures – Novel Therapeutics Discoveries Through Multidisciplinary Research, UiTM Shah Alam, Sep 3-5.
- **2012 |** Co-Organizer for the Computer-Aided Drug Design (CADD 2012) (Seminar & Workshop), UiTM Puncak Alam Campus, 3-7th Dec.
- **2011 |** Workshop on Genomics and Bioinformatics for Microbial Applications, UiTM Puncak Alam Campus, Oct 13.
- **2011 |** Workshop on Discovery Studio, UiTM Puncak Alam Campus, May 12.

COMMITTEE MEMBER

- **2018 |** Committee for 2nd International Symposium for Bioinformatics (InSyB2018), Perdana University-Serdang, 20-21 December.
- **2016 |** IBRO-APRC Associate School of Neuroscience 2016, Faculty of Pharmacy, UiTM Puncak Alam, 8-14th Aug (Publicity).
- **2016 |** International Conference on Computation for Science and Technology (ICCST2016), Langkawi Nov 3-4 (Publicity).
- **2011 |** EU-ASEAN Scientific Workshop on Computational Biology, Kuala Lumpur - Nov 28-29.
- **2011 |** International Conference on Bioinformatics (InCoB/ISCB-Asia 2011), Kuala Lumpur - Nov 30-Dec 2.
- **2011 |** Colloquium on Pharmaceutical Sciences, Faculty of Pharmacy UiTM - Oct 7.

TEACHING

TEACHING EXPERIENCE

Bachelor of Pharmacy (Hons), Faculty of Pharmacy, UiTM

- PHC644 Structure-based Drug Design
- PHC429 Pharmaceutical Biochemistry
- PHC504 Pharmaceutical Biotechnology & Engineering
- PHC425 Biostatistics & Calculus
- PHC454 Pharmaceutical Microbiology & Parasitology
- PHC450 Pharmaceutical Immunology
- PHC650 Drugs in Sports
- PHC566 & PHC567 Research (Final Year Thesis Project)

Course & Program Developer (Faculty of Pharmacy, UiTM)

- MSc Molecular Informatics in Drug Discovery.
- PHC644 Structure-based Drug Design.

SUPERVISING

SUPERVISION

Postgraduates

- PhD (main supervisor), 3 students (Graduated)
- MSc (main-supervisor), 3 students (on-going)
- PhD (co-supervisor), 1 students (on-going)
- MSc (co-supervisor), 1 students (on-going)

Undergraduate Final Year Projects

- BPharm, 4 students (on-going)
- BPharm, 24 students (graduated)

Industrial Training/Practical Students/Internship

- 2018-2023 Internship/Industrial Training: IR4.0 Modules for MAKERLAB UiTM: 90 students (completed)
- 2013 Management Science University (MSU), 2: students (completed)

TRAINER/INVITED SPEAKER

2022 | Invited Speaker - **The 4th International Conference on Bioscience & Medical Engineering (ICBME2022)**, organized by International Islamic University Malaysia (IIUM) June 21-22

2021 | Trainer - **A Sharing Session on 3D Modeling & Printing**, Department of Mechanical Engineering, organized by Politeknik Banting, June 2 - 2021.

2021 | Speaker - **A Sharing session on the Collaborative Group (CG) Makerspace**, organized by CIDL UiTM, March 12 - 2021.

2021 | Speaker - **A sharing session on Applications of Computer-Aided Drug Design Methods**, organized by Faculty of Pharmacy UiTM, March 10 - 2021.

2020 | Trainer - **3D Modelling & 3D Printing for the Science & Technology & Innovation (STI) Selangor 2020**, organized by Perbadanan Perpustakaan Awam Selangor (PPAS), Nov 28-29, 2021.

2020 | Invited Panel - **A Sharing session on Makerspace Best Practices in the University Library**, organized by PTAR UiTM Kampus Puncak Alam, Mei 21, 2021.

2018 | Trainer for **Molecular Docking Workshop - Seminar & Workshop Computer-Aided Drug Design (CADD 2018)**, Dec - Bali, Indonesia.

2018 | Trainer for **Workshop on Basic Molecular Docking**, Bioinformatics Lab, Faculty of Pharmacy, UiTM, April 6.

2017 | **Trainer for Molecular Docking Workshop** - Seminar & Workshop Computer-Aided Drug Design (CADD 2017), Langkawi.

2016 | Trainer for Workshop on Docking & Protein Modeling - 7th International Conference on Computational System-Biology and Bioinformatics (CSBio-2016), Dec 19-22. MACAU.

2015 | **Facilitator for BioChem Core Summer Program organized by** Amaro Group, University California San Diego, (UCSD), USA. Aug-Sep.

2013 | **Speaker for LRGS Dengue Colloquium & Workshop**, University of Malaya June 11-12.

2013 | **Trainer for Workshop on Protein Modeling & Docking**, 2-6 December. Bioinformatics Lab, Faculty of Pharmacy, UiTM Campus Selangor.

2013 | **Trainer for Workshop on Protein Structure Prediction for Diagnostics Application**, 28-30th May. Institute for Medical Research (IMR), Kuala Lumpur.

2013 | **Speaker for Workshop on "How to Write A Winning Grant Proposal"**, Faculty of Medicine UiTM, May 30-31.

2012 | **Trainer for Protein Structure Prediction Workshop**, 14-17th May. Malaysia Genome Institute (MGI), Bangi.

2011 | **Invited Speaker for International Symposium & Workshop on Functional Genomics and Structural Biology**, May 9-13.