Mohamed Marzouk Sobeh, Ph.D.

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Career Progression

Dec. 2016 - April 2019

■ Senior Teaching/Research Assistant

Physics Department, Faculty of Science, Ain Shams University, Cairo, Egypt.

Mar. 2010 - Dec. 2016

Junior Teaching/Research Assistant

Physics Department, Faculty of Science, Ain Shams University, Cairo, Egypt.v

Education

April 2019 – March 2022

Ph.D., School of Life Science and Technology, Tokyo Institute of Technology in Computational Biology.

Thesis title: Investigating Dissociation Process and Binding Free Energy of P53-DBD/DNA Complex by PaCS-MD and MSM.

June 2012 – October 2016

M.Sc.Faculty of Science, Ain Shams University in Biophysics.
Thesis title: Genetic and Physiological Effects of Ultraviolet Radiation on Tomato Plant (solanum lycopersicum).

September 2005 – June 2009

B.Sc.Faculty of Science, Ain Shams University in Biophysics.

Positions

April 2022 – present

Postdoctoral researcher, Molecular Modeling and Simulation (MMS) Team, National Institute for Quantum Science and Technology (QST), Chiba, Japan.

Project title: The Development of Basic Drug Discovery Technologies for the Production of Next-Generation Antibody Therapeutics.

Research Publications

Journal Articles

- **Sobeh**, **M. M.**, & Kitao, A. (2022). Dissociation pathways of the p53 DNA binding domain from DNA and critical roles of key residues elucidated by dPaCS-MD/MSM. *Journal of Chemical Information and Modeling*, 62(5), 1294–1307. Odi:10.1021/acs.jcim.1c01508
- Hata, H., Tran, D. P., **Sobeh**, **M. M.**, & Kitao, A. (2021). Binding free energy of protein/ligand complexes calculated using dissociation parallel cascade selection molecular dynamics and markov state model. *Biophysics and Physicobiology*, 18(0), 305–316. 6 doi:10.2142/biophysico.bppb-v18.037

Conference Proceedings

- Sobeh, M. M., Sakuraba, S., & Kono, H. (2022.11.14). Predicting the Effect of Addition/Deletion Mutations on Protein Stability by REST/FEP. In Proceedings of the Annual Meeting progress FY2022 of AMED Fundamental Drug Discovery Technology Development Project for Realising Next Generation Therapy and Diagnosis, Poster, Kobe University Integrated Research Centre, Kobe University, Japan.
- Sobeh, M. M. (2021.9.16). Investigating the dissociation process and binding free energy of the p53-DBD/DNA complex by PaCS-MD and MSM. In *Proceedings of The Third International Online Conference on Molecular Modeling and Spectroscopy*, Short presentation, Online Conference, Giza, Egypt. Retrieved from https://www.youtube.com/watch?v=wro0ofDsxos
- Sobeh, M. M., & Kitao, A. (2021.4.28). Investigating the dissociation process and binding energy of the p53-DBD/DNA complex by PaCS-MD and MSM. In *Proceedings of WE-Heraeus-Seminar, Advanced Physical and Computational Techniques to Investigate Protein Dynamics*, Poster, Online Conference via MeetAnyway, Freie Universität Berlin, Germany. Retrieved from https://shortest.link/2mnF
- **Sobeh**, **M. M.**, & Kitao, A. (2021.6.16). Investigating the dissociation process and binding free energy of the p53-DBD/DNA complex by PaCS-MD and MSM. In *Proceedings of the 21st Annual Meeting of the Protein Science Society of Japan*, Poster, Online Conference, Tokyo, Japan.
- **Sobeh**, **M. M.**, & Kitao, A. (2020.9.18). Investigating the dissociation process of the p53-DBD/DNA complex by PaCS-MD and MSM. In *Proceedings of The 58th Annual Meeting of Biophysical Society of Japan (BSJ)*, Poster, Online Conference, Tokyo, Japan.

Skills

Coding Python, Bash, Tcl, LaTeX, Git

MD Simulation & Analysis AMBER, GROMACS, VMD, PyMOL, Chimera, PLIP, Autodock vina, PyEMMA, MSMbuilder, Mdtraj, MDAnalysis, GitHub.

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Interpersonal Communication & Presentation skills, Ability to teach and mentor Strong administrative & organizational skills, Effective team member

Like water can adapt any situation and make better environment

Teaching Guiding students in performing the experiments and taking data Helping students to figure out assignment problems

Leading discussion sessions, Grading lab reports

Preparing/Grading exams and quizzes

Miscellaneous Experience

Professional Experiences

August, 2021 **Tokyo 2020 Paralympic Games**, Contribution as volunteer with Germany Media Team.

July, 2021 **Tokyo 2020 Olympic Games**, Contribution as volunteer with Austrian Media Team.

Awards and Achievements

2021 – 2022 Cross the border, Tokyo-Tech pioneering doctoral research program by Tokyo Institute of Technology.

2019 – 2021 **Tokyo Tech Tsubame Scholarship**, Tokyo Institute of Technology.

Ph.D. Scholarship, The Egypt-Japan Education Partnership (EJEP).

Miscellaneous Experience (continued)

Medal of Superiority, Awarded by dean of Faculty of Science, Ain Shams University, Cairo, Egypt.

Honor Certificate, Awarded by Egyptian Syndicate of Scientific Professions.

Cross the border! Tokyo-Tech pioneering doctoral research program" program

Workshops and Training

February, 2022 Fundamentals of Deep Learning, NVIDIA Deep Learning Institute.

June, 2021 Python Data and Scripting and Molecular Mechanics Tools, MolSSI Workshops offered at MERCURY Conference 2021.

BioExcel Summer School on Biomolecular Simulations, Centre of Excellence for Computational Biomolecular Research.

May, 2021 | **Python Package Development Workshop**, MolSSI Workshops.

March, 2021 Introduction to Simulation Environments for Life Sciences, Online PATC@BSC Training Course.

References

Available on Request