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## EDUCATION

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**Doctorate of Philosophy in Theoretical and Computational Chemistry** Spring 2023

Southern Methodist University, Dallas, TX, USA

Thesis: Protein Dynamics in Allostery and Computer-Aided Drug Design

**Bachelor of Biomedical Sciences in Drug Design and Development**

**Minor: Nanoscience**

Spring 2019

University of Science and Technology, Zewail City, Egypt

Thesis: Molecular Modeling and Database Mining to Find Inhibitors for Protein-Protein

Interaction Between MOAG-4/SERF 1A And aSyn: An Approach to Treat Parkinson's Disease

## EXPERIENCE

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**Computational Chemistry Intern** September 2022 - Present

SandboxAQ Company, Remote Position, USA

- Developed codes to apply machine learning techniques to advance the conventional computer-aided drug design, forcefield development, and quantum calculations.

**Graduate Research Assistant**

2019 - Present

Southern Methodist University, Dallas, TX, USA

- Studied the allosteric mechanism of LOV2 domains using molecular dynamics simulations and machine learning techniques. Investigated the applications of machine learning techniques to advance available computer aided-drug design techniques.

**Research Assistant**

August 2018 - July 2019

Drug Discovery Lab, Zewail City, Egypt

- Developed possible inhibitors targeting MOAG4/SERF 1A interaction in Parkinson's using CADD.

**Research Assistant**

July - August 2018

University of Florida, Gainesville, FL, USA

- Studied the kinetics of glutathione transferases in rat liver cytosol.

**Trainee**

August - September 2017

Multi Apex Pharmaceutical Company, Cairo, Egypt

- Shadowed employees in the research and development, quality assurance, and quality control departments.

**Research Assistant**

June - August 2016

Center of Aging and Associated Diseases, Zewail City, Egypt

- Investigated various pathways and their role in brain cancer through different molecular techniques including cell culture, Western blot and PCR.

**Research Assistant**

June - September 2015

Center of Excellence for Stem Cells and Regenerative Medicine, Zewail City, Egypt

- Studied the effect of estrogen on stem cells and its role in developing breast cancer.

## SKILLS

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Molecular Dynamics Simulations, Machine Learning, QM/MM, Artificial Intelligence, Python, Linux, HPC, Bash, TensorFlow, PyTorch, Ab-initio Calculations, ADME/TOX Calculations, Molecular Docking, Binding Free Energy Calculations, Pharmacophore Modelling, QSAR, Homology Modeling, Bioinformatics Basics, SPSS, Standard Microbiological Practices, and Molecular Biology Techniques

## ARTICLES & SCIENTIFIC REVIEWS

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Ibrahim, M.T., Verkhivker, G.M., Misra, J. & Tao, P. (2023) Novel allosteric effectors targeting human transcription factor TEAD, International Journal of Molecular Sciences, submitted

Ibrahim, M. T., & Tao, P. (2022) Computational investigation of peptidomimetics as potential inhibitors of SARS-CoV-2 spike protein. Journal of Biomolecular Structure and Dynamics, pp.1-14. doi: 10.1080/07391102.2022.2116601

Ibrahim, M.T., Lee, J. & Tao, P. (2022) Homology modeling of Forkhead box protein C2: identification of potential inhibitors using ligand and structure-based virtual screening. Mol Divers. doi: 10.1007/s11030-022-10519-0

Ibrahim, M. T., Trozzi, F., & Tao, P. (2022). Dynamics of hydrogen bonds in the secondary structures of allosteric protein Avena Sativa phototropin 1. Computational and structural biotechnology journal, 20, pp.50-64. doi: 10.1016/j.csbj.2021.11.038

Abdelbaky, S., Ibrahim, M. T., Samy, H., Mohamed, M., Mohamed, H., Mustafa, M., ... & Khalil, I. A. (2021). Cancer immunotherapy from biology to nanomedicine. Journal of Controlled Release. doi: 10.1016/j.jconrel.2021.06.025 [Review Article]

Ibrahim, M. T., Heba, A., Mostafa, N. and Shaimaa, A. (2017). Cell Signaling in Cancer Microenvironment. International Journal of Advanced Biomedicine, (2), pp.47 - 51. doi: 10.18576/ab/02020 [Review Article]

## AWARDS

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<b>People's Choice Award</b> , Three-Minute Thesis, Southern Methodist University	December 2020
<b>First Place</b> , Microbiology Competition, UST, Zewail City	January 2016
<b>First Place</b> , Biomedical Sciences Major, UST, Zewail City	Spring 2015

## INVITED SPEAKER

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<b>Applications of AI in Drug Design &amp; Development</b> Bioinformatics & Data Science Forum: Bioscience	November 2022
<b>Dynamics of hydrogen bonds in the allosteric protein of AsLOV2</b> Photosensory Receptors and Signal Transduction: Gordon Research Seminar	March 2022

## NOTABLE POSTERS

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Ibrahim, M. T., Trozzi, F., & Tao, P, Dynamics of hydrogen bonds in the secondary structures of allosteric protein Avena Sativa phototropin 1. Photosensory Receptors and Signal Transduction, Gordon Research Conference, Ventura, CA, March 2022.

Ibrahim, M. T., Zhao, T., & Tao, P, Protein dynamics and machine learning in Computer-Aided Drug Design, Women Make COMP symposium, Virtual ACS COMP, August 2021.

Ibrahim, M. T., Trozzi, F., & Tao, P, The structural role of A'α helix in AsLOV2, Virtual Conference on Theoretical Chemistry (VCTC), July 2020.